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Exact Thermal Boundary Conditions in 1d Heat Transport

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Kyle A Mylonakis

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June 2019

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Exact Thermal Boundary Conditions in 1d Heat Transport

“Hope clouds observation.”

– Frank Herbert, *Dune*

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Sample Code:

- `https://github.com/KyleMylonakis`

Abstract

Exact Thermal Boundary Conditions in 1d Heat Transport

by

Kyle A Mylonakis

It is well known that 1d atomistic heat transport experiences anomalous phenomenon. Temperature discontinuities and divergence of the conductivity with respect to system size suggest that, at the atomistic scale, Fourier's law does not hold in one dimensional materials. Many different thermostats exist for 1d atomistic systems, however their use is ad-hoc and requires choice of boundary conditions. A dimension reduction technique known as the Mori-Zwanzig procedure applied to infinite harmonic systems produces a type of thermostat whose equations of motion are generalized Langevin equations (GLE's) where the resulting noise term is mean zero Gaussian and stationary, satisfying the fluctuation dissipation theorem.

By using a dimension reduction procedure based on Green's function techniques, it is shown that infinite deterministic baths give rise to GLE thermostats with non-stationary noise. Numerical experiments are then performed to explore the affect of non-stationarity on the temperature profiles in non-equilibrium stationary states (NESS), and on the divergence of the conductivity. Comparisons to other simple models are also reported.

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Chapter 1

Introduction

1.1 Introduction

It is well understood that the presence of a temperature gradient can induce various physical currents. The practical applications of these currents can not be understated: For electric currents this is known as the Seebeck effect [2] and is used to power the Voyager spacecraft [65]. An analogous effect happens for the spins of a quantum mechanical system and is known as the Spin Seebeck effect [63]. As electronic devices become smaller and denser, the effect of heat becomes more important. Understanding the connection between temperature gradients at the atomic level and various currents could allow for more efficient control of the device.

Fourier's law states that the local heat flux of a system j is proportional to the gradient of the temperature ∇T:

$$j = -\kappa \nabla T. \tag{1.1}$$

The proportionality constant κ is the thermal conductivity of the system. For 3d materials, κ in general is a matrix. For extreme temperatures, κ itself may depend on temperature [66]. Fourier's law holds so well for such a wide class of materials at room temperature at the continuum level that heat and temperature are often colloquially considered the same phenomenon. This is not the case: the presence of a temperature gradient creates an energy current - the heat flux.

Because of the experimental validity of Fourier's law, an atomistic theory of heat would need to reproduce Fourier's law in the thermodynamic limit. To do this one would need a definition for the local temperature of a system out of equilibrium formulated at the level of classical or statistical mechanics. Unfortunately such a quantity is not easily defined, not the least of which is because temperature is inherently an equilibrium phenomenon [4]. As such, giving meaning to the quantities involved in Fourier's law is a challenge before even determining whether such a law would hold at such small scales.

Simple low dimensional models of atomistic heat transport are usually the only ones which admit analytic results. Yet, it is well known that physics in low dimensions often behaves significantly differently than in dimension three [41]. In particular, it is numerically observed that the thermal conductivity diverges as a function of the system size for one dimensional systems. This divergence has also been experimentally observed in solid polymers [22].

1.2 Models of Classical 1d Heat Transport

There are many models of atomistic 1d heat transport. Common to them all is the atomistic system of N particles interacting classically via some Hamiltonian $H(\mathbf{p}, \mathbf{q})$, $\mathbf{p}, \mathbf{q} \in \mathbb{R}^N$, where $\mathbf{q}$ represents positions of the particles, and $\mathbf{p}$ their momentum. A common simplification is to assume that particles only interact with their nearest neighbors. All models in this thesis will be assumed to have nearest neighbor interactions unless otherwise stated. Assuming this, the Hamiltonian has the form

$$H(\mathbf{p},\mathbf{q}) = \sum_{j=1}^{N+1} \frac{p_j^2}{2m_j} + \phi(q_j - q_{j-1}) \tag{1.2}$$

where m_j is the mass of the particle j. Typically one chooses periodic boundary conditions $q_0 = q_{N-1}, q_{N+1} = q_1$, free boundary conditions $\phi(q_1 + q_0) = 0, \phi(q_{N+1} + q_N) = 0$, or fixed boundary conditions $q_0 = q_N = 0$.

Temperature gradients are then added to the system by a choice of thermostat. Thermostats can be roughly divided into two categories: deterministic thermostats, where the thermostats are modeled by their own deterministic evolution, and stochastic thermostats, where noise is judiciously added. To study a non-equilibrium properties of a system at least two thermostats at different temperature must be added. The thermostats themselves can interact with one or more particles of the system.

Infinite Harmonic Baths

An analytically tractable model of one-dimensional heat transport is to couple a finite system of particles to two semi-infinite harmonic systems (systems whose interaction potential is nearest neighbor and quadratic). This is a deterministic thermostat with formal Hamiltonian

$$H = \frac{1}{2}\sum_{j\in\mathbb{Z}} p_j^2 + \sum_{j=1}^{N-1} \phi(q_{j+1} - q_j + a) + \sum_{\substack{j\leq 1,\\ j\geq N+1}} \frac{k^2}{2}(q_j - q_{j-1})^2. \tag{1.3}$$

Harmonic baths are known to have infinite thermal conductivity acting as thermal superconductors [58]. The infinite nature of the bath in principle allows for energy to escape to infinity without bouncing back or otherwise being scattered by finite conductivity, causing equilibriation. The infinitude of the bath is necessary to maintain a thermal gradient across the system but makes numerics and rigorous analysis challenging, but tractable [51].

Langevin Equation: Another common thermostat is to add white noise and damping to the forces acting on the boundaries of a 1d atomic chain. The resulting equations of motion are known as Langevin equations:

$$d\dot{q}_1 = (\phi'(q_1 - q_2) - \phi'(q_0 - q_1) - \lambda\dot{q}_1)\, dt + \sqrt{2\lambda T_L} dW_t^L, \tag{1.4}$$
$$\dot{q}_j = -\phi'(q_j - q_{j-1}) + \phi'(q_{j+1} - q_j) \quad , j = 2, \ldots, N-1, \tag{1.5}$$
$$d\dot{q}_N = (-\phi'(q_{N-1} - q_N) + \phi'(q_{N+1} - q_N) - \lambda\dot{q}_N)\, dt + \sqrt{2\lambda T_R} dW_t^R, \tag{1.6}$$

where T_L and T_R are the temperatures of the left and right baths, where λ_L and λ_R are damping parameters for the left and right baths, and where W_t^L and W_t^R are independent standard Weiner processes. The above stochastic differential equations are interpreted in the sense of Itô. Langevin thermostats offer a convenient numerically tractable way to add noise to a system. For simple potentials, they also offer closed form solutions, the simplest of which is the Ostein-Uhlenbeck process [46]. When fixed boundary conditions are chosen, the local kinetic temperature of the non-equilibrium stationary state (NESS) of the Langevin equation experiences anomalous behavior exhibiting constant temperature in the bulk with large discontinuities at the interfaces: see figure 1.1 on 5.

Generlized Langevin Equations:

The Langevin equation is a special case of the generalized Langevin equation (GLE):

$$\ddot{q}_1 = \phi'(q_2 - q_1) - \int_0^t \theta_L(t-s)\dot{q}_1(s)ds + F_L(t), \tag{1.7}$$
$$\ddot{q}_j = \phi'(q_{j+1} - q_j) - \phi'(q_j - q_{j-1}), \quad j = 2, \ldots, N-1, \tag{1.8}$$
$$\ddot{q}_N = -\phi'(q_{N-1} - q_N) - \int_0^t \theta_R(t-s)\dot{q}_N(s)ds + F_R(t), \tag{1.9}$$

where $F(t)$ is a noise term. The functions θ are called the memory kernels of the left and right baths. The GLE can be derived by applying the Mori-Zwanzig procedure to a finite system coupled to two infinite harmonic baths [67]. Using the Mori-Zwanzig approach, it is argued F is a mean zero stationary Gaussian process with correlation function satisfying the fluctuation dissipation theorem $\langle F(0)F(t)\rangle = k_B T\theta(t)$. One can

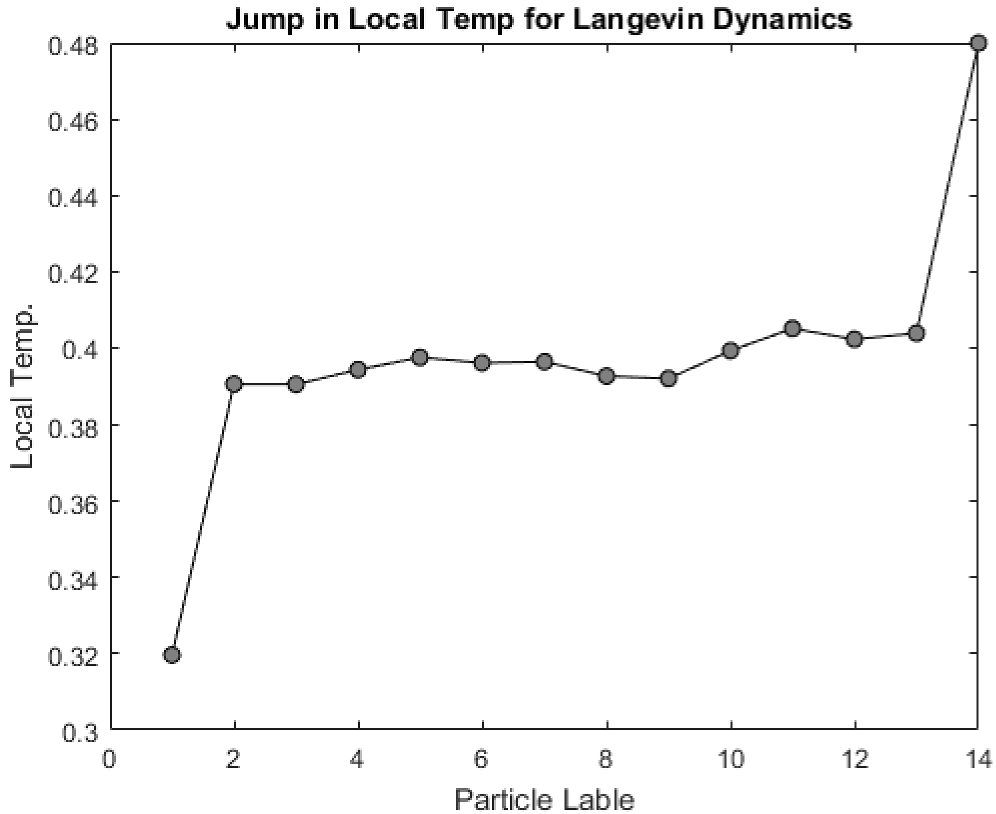


Figure 1.1: Langevin dynamics are run until the system equilibrates. The local temperature is computed as the average kinetic energy of each particles in the NESS.

formally recover the Langevin equation for the GLE by letting setting $\theta(t) = \delta(t)$, where $\delta(t)$ is the Dirac delta distribution, and maintaining the enforcement of the fluctuation dissipation theorem. While the equations of motion involve no stochastic integrals, they are still integrodifferential equations with noise.

Nosé-Hoover Thermostat

Another way to thermostat a system is to penalize deviations from the average temperature. This is accomplished in a deterministic non-Hamiltonian way by the Nosé-Hoover thermostat. Let I_L and I_R be the set of indices of particles interacting with the left and right baths respectively. Each particle is assumed to interact with at most one bath. The equations of motion of a Nosé-Hoover thermostat (representing the left bath) interacting with particle j is given by:

$$m_j\ddot{q}_j = -\phi'(q_j - q_{j-1}) + \phi'(q_{j+1} - q_j) - \eta_L \dot{q}_j, \tag{1.10}$$

$$\dot{\eta}_L = \frac{1}{\Theta_L^2}\left(-1 + \frac{1}{k_B T_L |I_L|}\sum_{k\in I_L} m_k \dot{q}_k{}^2\right), \tag{1.11}$$

where Θ_L is the left thermostat response time. The equations of motion of a particle interacting with the right reservoir have a similar form.

Gaussian Thermostats

By taking the singular limit of the Nosé-Hoover thermostat response time $\Theta \to 0$ one recovers the Gaussian thermostat [41]. In this limit one can solve for the additional dynamical variable η exactly:

$$\eta = \frac{\sum_{j\in I} \dot{q}_j \left[-\phi'(q_j - q_{j-1}) + \phi'(q_{j+1} - q_j)\right]}{\sum_{j\in I} \dot{q}_j^2}, \tag{1.12}$$

where I is the set of indexes of particles interacting the reservoir. This makes Gaussian thermostats easy to implement and computationally efficient, but is only appropriate for systems where the thermostat response time is very small.

Elastic Collisions and Thermal Walls

Another approach is to assume the boundary atoms are hard spheres undergoing elastic collisions. Times which the boundary particles collides with a particle from the baths (which are not being explicitly simulated) are randomly selected from a Poisson (exponential) distribution with chosen characteristic time τ. After colliding, the velocity of the boundary particles is then updated as

$$\dot{q} + \frac{2m}{m + m_R}(\dot{q}_R - \dot{q}), \tag{1.13}$$

where m_R and $\dot{q}_R$ are the mass and velocity of the interacting particle in the bath, and where the velocity $\dot{q}_R$ is selected from the equilibrium distribution:

$$\sqrt{\frac{\beta m_R}{2\pi}} \exp\left[-\beta \frac{m_R \dot{q}_R^2}{2}\right] \tag{1.14}$$

where $\beta = \frac{1}{k_B T}$ is the inverse temperature parameter. Between collisions the equations of motion are determined by the Hamiltonian 1.2. This method again is trivial to implement, and allows for the use of symplectic integrators between the collisions [41].

1.3 Relevant Observables and Anomalous Behavior

Ideally ensemble averages are performed in order to compute statistical properties of the dynamical system. These averages are often hard to perform, or entirely inaccessible. One instead assumes ergodicity of the system so that ensemble averages may be replaced with time averages, which are easily computed [40, 41].

Throughout the remainder of the section, suppose we have a 1d system $\mathbf{q}(t), \mathbf{p}(t) : \mathbb{R}^+ \to \Gamma = \mathbb{R}^N \times \mathbb{R}^N$ where $\dot{\mathbf{q}} = \mathbf{p}$ of N particles interacting classically with a nearest neighbor interaction potential $\phi : \mathbb{R} \to \overline{\mathbb{R}}$. Fix some time $T > 0$ and a time step $\Delta t > 0$. Let $S = \{(\mathbf{q}(T + j\Delta t), \mathbf{p}(T + j\Delta t) : j = 0, \ldots N\}$ be the set of uniformly spaced samples of the dynamical system starting at time T.

Definition 1.1. *The empirical local kinetic temperature of the j^{th} particle, or local temperature for short, is defined to be*

$$T_j := \frac{1}{|S|} \sum_{(\mathbf{q},\mathbf{p}) \in S} p_j^2, \tag{1.15}$$

where $|S|$ denotes the number of particles in S.

Definition 1.2. *The local energy of particle j is the function $h_j : \Gamma \to \mathbb{R}$*

$$h_j(\mathbf{q}, \mathbf{p}) = \frac{1}{2}\left[p_j^2 + \phi(q_{j+1} - q_j) + \phi(q_j - q_{j-1})\right] \text{ for } , j = 2, \ldots, N-1 \tag{1.16}$$

$$h_1(\mathbf{q},\mathbf{p}) = \frac{1}{2}\left[p_1^2 + \phi(x_2 - x_1)\right], \tag{1.17}$$

$$h_N(\mathbf{q},\mathbf{p}) = \frac{1}{2}\left[p_N^2 + \phi(x_N - x_{N-1})\right]. \tag{1.18}$$

Definition 1.3. *The empirical local heat flux of particle i through particle $i+1$, or local heat flux for short, is defined to be*

$$j_i = \frac{1}{|S|}\sum_{(\mathbf{q},\mathbf{p})\in S} -\frac{1}{2}(q_{i+1} - q_i)(p_{i+1} + p_i)\phi'(q_{i+1} - q_i) + p_i h_i, \tag{1.19}$$

where $h_i = h_i(\mathbf{q},\mathbf{p})$ for $i = 1, \dots N-1$.

Definition 1.4. *The empirical local heat flux in the limit of small oscillations of particle i, or local heat flux in the small oscillation limit for short, is defined to be*

$$j_i^o = \frac{1}{|S|}\sum_{(\mathbf{q},\mathbf{p})\in S} -\frac{1}{2}a(p_{i+1} + p_i)\phi'(q_{i+1} - q_i), \tag{1.20}$$

where $a = \arg\min_{x\in\mathbb{R}^+} \phi(x)$, assuming it exists for the chosen potential ϕ.

Definition 1.5. *The total heat flux is defined (resp. total heat flux in the limit of small oscillations) to be*

$$J = \sum_{i=1}^{N} j_i \quad \left(\textit{resp. } J^o = \sum_{i=1}^{N} j_i^o \right). \tag{1.21}$$

Definition 1.6. *The thermal conductivity (resp. thermal conductivity in the limit of small oscillations) of the system is defined to be*

$$\kappa = \frac{JN}{T_N - T_1} \quad \left(\textit{resp. } \kappa^o = \frac{J^o N}{T_N - T_1} \right), \tag{1.22}$$

Definition 1.7. *The conductivity (resp. conductivity in the limit of small oscillations) growth rate, or conductivity scaling coefficient, is defined to be the* $\alpha \in \mathbb{R}$ *(resp.* $\alpha^o \in \mathbb{R}$ *) such that*

$$\kappa(N) = cN^{\alpha} \quad \left(\textit{resp. } \kappa^o(N) = cN^{\alpha^o} \right), \tag{1.23}$$

where $c \in \mathbb{R}$ *is an arbitrary constant and* $N \in \mathbb{N}$ *is the system size, assuming such* α *and* α^o *exist.*

Definition 1.8. *The conductivity (resp. conductivity in the limit of small oscillations) truncation scaling coefficient, is defined to be the* $\beta \in \mathbb{R}$ *(resp.* $\beta^o \in \mathbb{R}$ *) such that*

$$\kappa(N) = cT^{\beta} \quad \left(\textit{resp. } \beta^o(T) = cT^{\beta^o} \right), \tag{1.24}$$

where $c \in \mathbb{R}$ *is an arbitrary constant and* $T \in \mathbb{N}$ *is the system size and* T *is the truncation parameter defined in definition 6.10.*

Detailederivations for all but definition 1.8 are presented in [41].

1.4 Formal Reduction of Infinite Harmonic Baths by Green's Functions

Consider the following bi-infinite one dimensional system of unit mass classical neutrally charged particles. This system is made up of three subsystems: a left thermal bath, a center resolved system, and a right thermal bath. All three subsystems are considered to be non-interacting until an initial specified time, for convenience to be thought of as $t = 0$. The baths are assumed to be independently in equilibrium at temperatures T_L and T_R respectively at $t = 0$.

Definition 1.9. *The equilibrium point of the Lennard-Jones potential is*

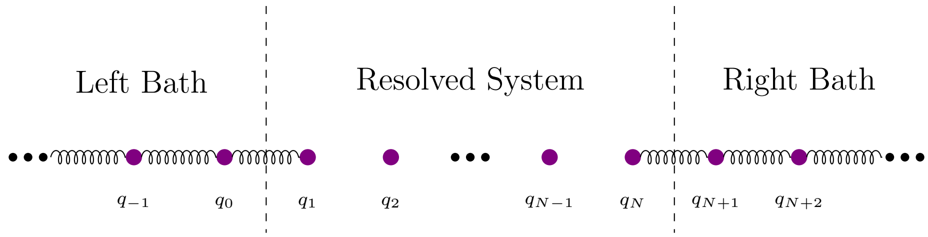


Figure 1.2: The one-dimensional system. The q_i denote the positions of particle i. The springs represent harmonic coupling and the blanks represent nearest neighbor Lennard-Jones coupling.

$$a = \arg\min_{x\in\mathbb{R}^+} x^{-12} - x^{-6}. \tag{1.25}$$

Definition 1.10. *The confined Lennard-Jones potential is*

$$\phi(x) = x^{-12} - x^{-6} + 4(x-a)^3. \tag{1.26}$$

Definition 1.11. *The constant $k \in \mathbb{R}^+$ is defined by $k^2 = \phi''(a)$.*

The system described has the following formal Hamiltonian:

Definition 1.12. *The formal Hamiltonian of the full bi-infinite system is*

$$H(\mathbf{q},\mathbf{p}) = \underbrace{\frac{1}{2}\sum_{j\in\mathbb{Z}} p_j^2}_{\text{Kinetic Energy}} + \underbrace{\sum_{j=1}^{N-1}\phi(q_{j+1}-q_j)}_{\substack{\text{Potential Energy}\\ \text{of the Resolved System}}} + \underbrace{\sum_{\substack{j\le 1,\\ j\ge N+1}} \frac{k^2}{2}(q_j - q_{j-1})^2}_{\substack{\text{Potential Energy}\\ \text{of the Baths}}} \tag{1.27}$$

where q_j and p_j are the position and momentum (velocity) of particle j, and where $\mathbf{q},\mathbf{p} \in \mathbb{R}^{\mathbb{Z}}$ are the vectors of position and momentum respectively.

Unfortunately this Hamiltonian is infinite unless the velocities of the particles decay to zero sufficiently fast at infinity, which is physically unreasonable.

Definition 1.13. *The displacement of the infinite system at time t, is defined to be the function $u : [0,\infty) \to \mathbb{R}^{\mathbb{Z}}$. The displacement of particle j is denoted u_j.*

Definition 1.14. *The position of particle j is defined to be $q_j = u_j + ja$. The function $q : [0, \infty) \to \mathbb{R}^\infty$ is the position of the system.*

Definition 1.15. *The total number of resolved particles is given by the fixed natural number $N \geq 2$.*

Definition 1.16. *The left (resp. right) bath are the particles with index $j \leq 0$ (resp. $j \geq N+1$).*

Definition 1.17. *The resolved system are the particles with index $j = 1, \dots N$*

The time evolution of the displacement satisfies Newton's laws of motion. In the baths these are

$$\ddot{u}_j = -k^2(-u_{j+1} + 2u_j - u_j), \quad j \leq 0, j \geq N+1, \tag{1.28}$$

where k^2 is defined in 1.11. If we define the discrete Laplace operator by $\mathcal{L} : \mathbb{R}^{\mathbb{Z}} \to \mathbb{R}^{\mathbb{Z}}$ by $\mathcal{L}(u_j) = k^2(-u_{j+1} + 2u_j - u_j)$, then we may write the dynamics in the baths as

$$\ddot{u}_j = -\mathcal{L}u_j, \quad j \leq 0, j \geq N+1. \tag{1.29}$$

Definition 1.18. *The Laplace transform of a function $h : \mathbb{R}^+ \to \mathbb{R}$ at a point $s \in \mathbb{C}$ is defined to be*

$$H(s) = \int_0^\infty h(t)e^{-st}dt, \tag{1.30}$$

assuming the integral exists.

Taking the Laplace transform of the odes for the bath (1.28), gives the set of difference equations

$$-\dot{u}_j(0) - su_j(0) + k^2(-U_{j+1}(s) + (s^2+2)U_j(s) - U_{j-1}(s)) = 0, \quad j \leq 0, j \geq N+1, \tag{1.31}$$

where

$$U_j(s) = \int_0^\infty u_j(t)e^{-st}dt.$$

Definition 1.19. *Set* $f_j(s) := \dot{u}_j(0) + su_j(0)$.

Taking the Laplace transform of the set of finite difference equations in the baths yields

$$(s^2 + \mathcal{L})U_j(s) = f_j(s) \quad j \leq 0, j \geq N+1. \tag{1.32}$$

The strategy will be to solve this system through the use of Green's functions.

Definition 1.20. *For each* $i \in \mathbb{Z}$ *let* $g_i(t)$ *be the solution to the set of ODE's*

$$\ddot{g}_{ij} = -\mathcal{L}g_{ij}, \quad j \in \mathbb{Z}, \tag{1.33}$$
$$\dot{g}_{ij}(0) = \delta_{ij}, \quad j \in \mathbb{Z}, \tag{1.34}$$
$$g_{ij}(0) = 0, \quad j \in \mathbb{Z}, \tag{1.35}$$

where for notational convenience $g_{ij} := (g_i)_j$, *and* δ_{ij} *is the Kronecker delta.*

Definition 1.21. *The Laplace transform of* g_{ij} *is defined to be* G_{ij}.

Taking the Laplace transform, the equations 1.20 become

$$(s^2 + \mathcal{L})G_{ij} = \delta_{ij} \quad j \leq 0, j \geq N+1. \tag{1.36}$$

We suppress the dependence of the U's and G's on s for notational convenience. Returning to the dynamics in Laplace space (1.32), for each $i \leq 0$ and $i \geq N+1$, if we multiply each each equation in j by G_{ij}, and sum over all the non-positive j we arrive at

$$\sum_{j\leq 0} G_{ij}(s^2 + \mathcal{L})U_j = \sum_{j \leq 0} G_{ij} f_j. \tag{1.37}$$

At the moment, convergence of the sum on the right hand side is not discussed and considered a formal sum, however it will be shown in future sections that the decay in j of the Green's functions cause it to converge in some (probabilistic) sense. Since the all the f_j are linear combinations of the initial conditions, if one can solve for the Green's function G_{ij}, then the right hand side of the above equation is a known quantity. The left hand side may be rewritten using summation by parts:

$$\begin{aligned}
&\sum_{j\leq 0} G_{ij}(s^2+\mathcal{L})U_j \\
&= \sum_{j\leq 0} G_i j(-k^2U_{j+1}+(2k^2+s^2)U_j-k^2U_{j-1}) \\
&= -k^2G_{i0}U_1+k^2G_{i1}U_0+\sum_{j\leq 0}(-k^2G_{i(j-1)}+(s^2+2k^2)G_{ij}-k^2G_{i(j+1)})U_j \\
&= -k^2G_{i0}U_1+k^2G_{i1}U_0+\sum_{j\leq 0}((s^2+\mathcal{L})G_{ij})U_j \\
&= -k^2G_{i0}U_1+k^2G_{i1}U_0+\sum_{j\leq 0}\delta_{ij}U_j \\
&= -k^2G_{i0}U_1+k^2G_{i1}U_0+U_i
\end{aligned}$$

After rearranging

$$U_i = k^2G_{i0}U_1 - k^2G_{i1}U_0 + \sum_{j\leq 0} G_{ij}f_j.$$

We can use this to get a boundary condition for the left bath:

$$U_0 = \frac{k^2G_{00}U_1}{1+k^2G_{01}} + \sum_{j\leq 0}\frac{G_{0j}f_j}{1+k^2G_{01}}. \tag{1.38}$$

If one could solve the Green's functions explicitly and sample the initial positions and momentums in the bath, then equation (1.38) on page 13 expresses U_0 in terms of U_1 and known quantities. This formula suggests the following definitions:

Definition 1.22. *The displacement memory kernel is the function $\beta(t)$ which is defined by its Laplace transform $\tilde{\beta}$,*

$$\tilde{\beta} = \frac{k^2 G_{00}}{1 + k^2 G_{01}}. \tag{1.39}$$

Definition 1.23. *The contribution of the bath as noise is the function $F(t)$, which is defined by its Laplace transform $\tilde{F}$,*

$$\tilde{F} = \sum_{j \le 0} \frac{G_{0j} f_j}{1 + k^2 G_{01}}. \tag{1.40}$$

Remark. *Throughout there are terms, such as the noise and memory, which must be defined for both the left and right baths independently. As such the subscripts L and R will be used to denote that this particular variable is referencing the left or right bath respectively. If no subscript is specified then that variable may be in reference to either bath, up to reindexing. For example F_L the noise contribution of the left bath, while F refers to the noise contribution of either bath.*

Inverting the Laplace transforms then would give that

$$u_0(t) = \int_0^t \beta_L(t-s) u_1(s) ds + F_L(t). \tag{1.41}$$

A similar derivation can be carried out for the right bath. Since both baths are coupled harmonically to the resolved system, the set of ODEs for the resolved system becomes

$$\ddot{u}_1 = \phi'(u_2 - u_1 + a) - k^2(u_1 - u_0), \tag{1.42}$$
$$\ddot{u}_j = \phi'(u_{j+1} - u_j + a) - \phi'(u_j - u_{j-1} + a), \quad j = 2, \ldots, N-1 \tag{1.43}$$
$$\ddot{u}_N = -\phi'(u_{N-1} - u_N + a) + k^2(u_{N+1} - u_N + a). \tag{1.44}$$

However, we have explicitly solved for u_{N+1} and u_0 in terms of the resolved system. This gives us the following system of equations:

$$\ddot{u}_1 = \phi'(u_2 - u_1 + a) - k^2 u_1 + k^2 \int_0^t \beta_L(t-s) u_1(s) ds + k^2 F_L(t), \tag{1.45}$$

$$\ddot{u}_j = \phi'(u_{j+1} - u_j + a) - \phi'(u_j - u_{j-1} + a), \quad j = 2, \ldots, N-1 \tag{1.46}$$

$$\ddot{u}_N = -\phi'(u_{N-1} - u_N + a) - k^2 u_N + k^2 \int_0^t \beta_R(t-s) u_N(s) ds + k^2 F_R(t). \tag{1.47}$$

To make this system of equations look like a generalized Langevin equation at the boundaries we make the following definition:

Definition 1.24. *The memory kernel θ is defined as*

$$\theta(t) = \int_t^\infty \beta(s) ds. \tag{1.48}$$

Then $\theta'(t) = -\beta(t)$, assuming β decays at infinity. Integrating by parts then gives

$$\int_0^t \beta_L(t-s) u_1(s) ds = \theta_L(0) u_1(t) - \theta_L(t) u_1(0) - \int_0^t \theta_L(t-s) \dot{u}_1(s) ds.$$

Similarly for the right bath we have

$$\int_0^t \beta_R(t-s) u_N(s) ds = \theta_R(0) u_N(t) - \theta_R(t) u_1(0) - \int_0^t \theta_R(t-s) \dot{u}_N(s) ds.$$

This transforms our set of integrodifferential equations for the bath into

$$\begin{aligned}
\ddot{u}_1 &= \phi'(u_2 - u_1 + a) - k^2 u_1(t) + k^2 \theta_L(0) u_1(t) - k^2 \theta_L(t) u_1(0), \\
&\quad - k^2 \int_0^t \theta_L(t-s) \dot{u}_1(s) ds + k^2 F_L(t) \\
\ddot{u}_j &= \phi'(u_{j+1} - u_j + a) - \phi'(u_j - u_{j-1} + a), \quad j = 2, \ldots, N-1, \\
\ddot{u}_N &= -\phi'(u_{N-1} - u_N + a) - k^2 u_N(t) + k^2 \theta_R(0) u_N(t) - k^2 \theta_R(t) u_1(0) \\
&\quad - k^2 \int_0^t \theta_R(t-s) \dot{u}_N(s) ds + k^2 F_R(t).
\end{aligned}$$

If $\theta_L(0) = \theta_R(0) = 1$, then the system reduces further to

$$\ddot{u}_1 = \phi'(u_2 - u_1 + a) - k^2\theta_L(t)u_1(0) - k^2 \int_0^t \theta_L(t-s)\dot{u}_1(s)ds + k^2 F_L(t) \tag{1.49}$$

$$\ddot{u}_j = \phi'(u_{j+1} - u_j + a) - \phi'(u_j - u_{j-1} + a), \quad j = 2, \ldots, N-1 \tag{1.50}$$

$$\ddot{u}_N = -\phi'(u_{N-1} - u_N + a) - k^2\theta_L(t)u_1(0) - k^2 \int_0^t \theta_R(t-s)\dot{u}_N(s)ds + k^2 F_R(t). \tag{1.51}$$

In order to formalize the above reduction, one must solve for the Green's functions in an appropriate function space, and then use them to prove convergence in some sense of the infinite sum defining the noise. This also requires constructing an equilibrium measure on the baths and determining the statistical properties of the initial bath degrees of freedom.

The remainder of the thesis is organized as follows. In Chapter 2, the equilibrium measure on the baths is constructed, and the statistical properties of the initial conditions of the bath degrees of freedom are found. In Chapters 3 we derive useful expressions for the Green's functions. In Chapter 4 we prove an expression for $\tilde{F}$, establishing convergence of the infinite sums in a probabilistic sense. Further, a relationship between the memory kernel and the noise terms is proved and used to establish non-stationarity of the noise. In Chapter 5 we prove global in time existence of solutions to systems similar to the reduced equations of motions, and other systems of interest. In Chapter 6 we perform numerical experiments to investigate various observables of the resolved system as well as other related systems. Concluding remarks are given in Chapter 7.

Chapter 2

Construction of the Baths

In order to evaluate the noise term in definition 1.23 on page 14, the initial conditions of the bath degrees of freedom must be sampled from an equilibrium measure on a space representing infinitely many classical particles interacting harmonically.

2.1 Construction and Properties of the Measure

Throughout it is taken as convention $\mathbb{Z}^-$ to be the set of non-positive integers, $\mathbf{e}_k$ to be a standard basis vector on $\mathbb{R}^{\mathbb{Z}^-}$, x_k to be the k-th coordinate of $\mathbf{x} \in \mathbb{R}^{\mathbb{Z}^-}$, and $\langle \cdot, \cdot \rangle$ to be the standard inner product on $\mathbb{R}^{\mathbb{Z}^-}$.

Definition 2.1. *For every $\mathbf{x} \in \mathbb{R}^\infty$ and for every $k \in \mathbb{Z}$, we denote the k-th component of $\mathbf{x}$ by $x_k = \langle \mathbf{x}, \mathbf{e}_k \rangle$, where $\mathbf{e}_k$ is the k-th standard basis vector and $\langle \cdot, \cdot \rangle : \mathbb{R}^\infty \times \mathbb{R}^Z \to \overline{\mathbb{R}}$ is the standard inner product.*

Definition 2.2. *Let $\langle \cdot, \cdot \rangle_\Delta : \mathbb{R}^{\mathbb{Z}^-} \times \mathbb{R}^{\mathbb{Z}^-} \to \overline{\mathbb{R}}$ be given by*

$$\langle \mathbf{x}, \mathbf{y} \rangle_\Delta = \lim_{N \to -\infty} \left\langle (2x_0 {-}_1)\mathbf{e}_0 + \sum_{i=-1}^{N+1} (-x_{i+1} + 2x_i - x_{i-1})\mathbf{e}_i + (2x_N - x_{N-1})\mathbf{e}_N, \right.$$
$$\left. \sum_{k=0}^{N} y_i \mathbf{e}_i \right\rangle .$$

Proposition 2.1. *The function* $\langle \cdot, \cdot \rangle_\Delta$ *is an inner product on*

$$\tilde{H} = \left\{ \mathbf{x} \in \mathbb{R}^{\mathbb{Z}^-} : \forall \mathbf{x}, \lim_{\text{N}\to\text{-}\infty} x_N < \infty, \langle \mathbf{x}, \mathbf{x} \rangle_\Delta < \infty \right\}.$$

Proof. By construction $\langle \cdot, \cdot \rangle_\Delta$ is bilinear and well defined, so to check that we have an inner product it suffices to check symmetry and positive definiteness. Both are checked with the following direct computations:

$$\begin{aligned}
\langle \mathbf{x}, \mathbf{y} \rangle_\Delta = &\lim_{N\to-\infty} (2x_0 - x_{-1})y_0 + \sum_{k=-1}^{N+1} (-x_{i+1} + 2x_i - x_{i-1})y_i \\
&+ (2x_N - x_{N-1})y_N \\
= &\lim_{\text{N}\to\text{-}\infty} 2x_0y_0 - x_1y_0 + \sum_{j=-2}^{N} (-x_{j+2}y_{j+1} + 2x_{j+1}y_{j+1} - x_jy_{j+1}) + 2x_Ny_N - x_{N+1}y_N \\
&= \lim_{\text{N}\to\text{-}\infty} (2y_0 - y_{-1})x_0 + \sum_{j=-2}^{N} (-y_{j+2} + 2y_{j+1} - y_j)x_{j+1} + 2x_Ny_N - x_{N-1}y_N \\
&= \lim_{\text{N}\to\text{-}\infty} (2y_0 - y_{-1})x_0 + \sum_{j=-2}^{N} (-y_{j+2} + 2y_{j+1} - y_j)x_{j+1} + (2y_N - y_{N-1})x_N \\
&= \langle \mathbf{y}, \mathbf{x} \rangle_\Delta,
\end{aligned}$$

where we used the fact that $\lim_{\text{N}\to\text{-}\infty} x_Ny_{N-1} = \lim_{\text{N}\to\text{-}\infty} x_{N-1}y_N$. This establishes symmetry. For positive definiteness we see that

$$\begin{aligned}
\langle \mathbf{x}, \mathbf{x} \rangle_\Delta &= \lim_{\text{N}\to\text{-}\infty} (2x_0 - x_{-1})x_0 + \sum_{i=-1}^{N+1} (-x_{i+1} + 2x_i - x_{i-1})x_i + (2x_N - x_{N+1})x_N \\
&= \lim_{\text{N}\to\text{-}\infty} x_0^2 + \left(\sum_{i=0}^{N+1} (x_i - x_{i-1})^2 \right) + x_N^2 \geq 0,
\end{aligned}$$

and further when $\langle \mathbf{x}, \mathbf{x} \rangle_\Delta = 0$ we get that $\lim_{\text{N}\to\text{-}\infty} x_N^2 = 0$, $x_0 = 0$, and $x_i = x_{i-1}$ for all $i \leq 0$, giving that $x = 0$. □

Definition 2.3. *Let* $(H, \langle, \rangle_\Delta)$ *be the smallest by inclusion Hilbert space containing* $(\tilde{H}, \langle, \rangle_\Delta)$.

Definition 2.4. *The norm of $x \in H$ is defined by $|| \mathbf{x} ||_{\Delta}^2 = \langle \mathbf{x}, \mathbf{x} \rangle_{\Delta}$.*

It will be important to understand the displacement of a particular particle in any given configuration. First we must choose an orthonormal basis for H.

Lemma 2.2. *For $n \leq 0$, the vectors*

$$\hat{\mathbf{u}}_n = \sqrt{\frac{1}{|n-2||n-1|}} \left(\mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |n-1| \mathbf{e}_n \right) \tag{2.1}$$

form an orthonormal basis for H.

Proof. The proof is by induction and uses the Gram-Schmidt orthonormalization procedure. Choose $\mathbf{u}_0 = \mathbf{e}_0$ and normalize to get $\hat{\mathbf{u}}_0 = \frac{1}{\sqrt{2}} \mathbf{e}_0$. This establishes the base case. Now fix $n \leq 0$ and suppose

$$\hat{\mathbf{u}}_m = \frac{1}{\sqrt{|m-1||m-2|}} \left(\mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |m-1| \mathbf{e}_m \right)$$

for all $m = 0, -1, \ldots, n$. The Gram-Schmidt orthonormalization results in

$$\mathbf{u}_{n-1} = \mathbf{e}_{n-1} - \langle \hat{\mathbf{u}}_n, \mathbf{e}_{n-1} \rangle_{\Delta} \hat{\mathbf{u}}_n - \cdots - \langle \hat{\mathbf{u}}_0, \mathbf{e}_{n-1} \rangle_{\Delta} \hat{\mathbf{u}}_0.$$

Calculating each term

$$\begin{aligned} \langle \hat{\mathbf{u}}_m, \mathbf{e}_{n-1} \rangle_{\Delta} = \langle \mathbf{e}_{n-1}, \hat{\mathbf{u}}_m \rangle_{\Delta} &= \langle -\mathbf{e}_n + 2\mathbf{e}_{n-1} - \mathbf{e}_{n-2}, \hat{\mathbf{u}}_m \rangle = -\langle \mathbf{e}_n, \hat{\mathbf{u}}_m \rangle \\ &= -\delta_{mn} \left(\frac{1}{\sqrt{|n-1||n-2|}} |n-1| \right) = -\delta_{mn} \sqrt{\frac{|n-1|}{|n-2|}}. \end{aligned}$$

Using this

$$\begin{aligned} \mathbf{u}_{n-1} &= \mathbf{e}_{n-1} + \sqrt{\frac{|n-1|}{|n-2|}} \hat{\mathbf{u}}_n \\ &= \mathbf{e}_{n-1} + \sqrt{\frac{|n-1|}{|n-2|}} \left[\frac{1}{\sqrt{|n-1||n-2|}} \left(\mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |n-1| \mathbf{e}_n \right) \right] \\ &= \mathbf{e}_{n-1} + \frac{1}{|n-2|} \left(\mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |n-1| \mathbf{e}_n \right). \end{aligned}$$

Computing $||\mathbf{u}_{n-1}||_\Delta$

$$\begin{aligned}
&||\mathbf{u}_{n-1}||_\Delta^2 \\
= &\left\langle \frac{1}{|n-2|}(2(1)-2)\mathbf{e}_0 + \sum_{j=-1}^{N+1} \frac{-|j+1|+2|j|-|j-1|}{|n-2|}\mathbf{e}_j + \left(-\frac{|n-1|}{|n-2|}+2\right)\mathbf{e}_{n-1}, \right. \\
&\left. \mathbf{e}_{n-1} + \frac{1}{|n-2|}\left(\mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |n-1|\mathbf{e}_n\right)\right\rangle \\
&= 2 - \frac{|n-1|}{|n-2|} = \frac{2|n-2|-|n-1|}{|n-2|} = \frac{|n-3|}{|n-2|},
\end{aligned}$$

and so

$$\begin{aligned}
\hat{\mathbf{u}}_{n-1} &= \sqrt{\frac{|n-2|}{|n-3|}}\left(\mathbf{e}_{n-1} + \frac{1}{|n-2|}\left[\mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |n-1|\mathbf{e}_n\right]\right) \\
&= \sqrt{\frac{1}{|n-2||n-3|}}\left[\mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |n-1|\mathbf{e}_n + |n-2|\mathbf{e}_{n-1}\right],
\end{aligned}$$

completing the induction. We now need to see whether this orthonormal family $\{\hat{\mathbf{u}}_n\}_{n=0}^{-\infty}$ is a basis for H. Fix $\mathbf{x} \in H$ with $\langle \mathbf{x}, \hat{\mathbf{u}}_n\rangle_\Delta = 0$ for all $n \in \mathbb{Z}^-$. We proceed by induction to prove that for each $m \leq 0$, $x_m = |m-1|x_0$. For the base case note that

$$\langle \mathbf{x}, \hat{\mathbf{u}}_0\rangle = \left\langle \mathbf{x}, \frac{1}{\sqrt{2}}\mathbf{e}_0\right\rangle_\Delta = \left\langle (2x_0 - x_{-1})\mathbf{e}_0, \frac{1}{\sqrt{2}}\mathbf{e}_0\right\rangle = 0$$

establishing $2x_0 = x_{-1}$. Further,

$$\langle \mathbf{x}, \hat{\mathbf{u}}_m\rangle = \langle \mathbf{x}, \mathbf{e}_0 + 1\mathbf{e}_{-1} + \cdots + |m-1|\mathbf{e}_m\rangle_\Delta = 0.$$

Fix m and assume that $|n-1|x_0 = x_n$ for all $m \leq n$. Then

$$\begin{aligned}
0 = &\left\langle (2x_0 - x_{-1})\mathbf{e}_0 + \sum_{i=-1}^{m+1}(-x_{i+1} + 2x_i - x_{i-1})\mathbf{e}_i + (-x_{m+1} + 2x_m - x_{m-1})\mathbf{e}_m, \right. \\
&\left. \mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |m-1|\mathbf{e}_m \right\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \Big\langle 0\mathbf{e}_0 + \sum_{i=-1}^{m+1}(-|i| + 2|i-1| - |i-2|)x_0\mathbf{e}_i + ((-|m| + 2|m-1|)x_0 - x_{m-1})\mathbf{e}_m, \\
&\mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |m-1|\mathbf{e}_m\Big\rangle \\
&= \Big\langle \sum_{i=-1}^{m+1}(-|i| + 2|i| + 2 - |i| - 2)x_0\mathbf{e}_i + ((2|m| + 2 - |m|)x_0 - x_{m-1})\mathbf{e}_m, \\
&\qquad \mathbf{e}_0 + 2\mathbf{e}_{-1} + \cdots + |m-1|\mathbf{e}_m\Big\rangle \\
&= \langle (|m-2|x_0 - x_{m-1})\mathbf{e}_m, |m-1|\mathbf{e}_m\rangle \\
&= |m-1|(|m-2|x_0 - x_{m-1}).
\end{aligned}
$$

This gives that $x_{m-1} = |m-2|x_0$, completing the induction. With this established we now see that if $\langle \mathbf{x}, \hat{\mathbf{u}}_m\rangle_\Delta = 0$ for all m, then since $x \in H$ gives $\lim_{\text{N}\to\text{-}\infty} x_N < \infty$, we must have $\lim_{\text{N}\to\text{-}\infty} |N-1|x_0 = 0$, which in turn yields $x_0 = 0$, and thus $x_m = 0$ for all m. Thus $\langle \mathbf{x}, \hat{\mathbf{u}}_m\rangle = 0$ for all m implies $x = 0$. This establishes that $\{\hat{\mathbf{u}}_m\}_{m=0}^{-\infty}$ is an orthonormal basis for H. □

Ultimately we want to understand how to represent the displacement of individual particles. We know that the displacement of particle j in terms of $\langle -, \hat{\mathbf{u}}_m\rangle_\Delta$.

Lemma 2.3. *The position of particle* 0 *is given by*

$$
x_0 = \lim_{\text{N}\to\text{-}\infty} \frac{1}{|N-2|} \sum_{j=0}^{N} |N-j-1| \langle \mathbf{x}, \mathbf{e}_j\rangle_\Delta. \tag{2.2}
$$

Proof. First we establish by induction the following: for all $n \le -1$

$$
x_0 = \frac{1}{|n-1|}\left[|n|\langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta + |n+1|\langle \mathbf{x}, \mathbf{e}_{-1}\rangle_\Delta + \cdots + \langle \mathbf{x}, \mathbf{e}_{n+1}\rangle_\Delta\right] + \frac{1}{|n-1|}\langle \mathbf{x}, \mathbf{e}_n\rangle.
$$

To establish the base case, by definition 2.2 on page 17

$$
\langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta = 2x_0 - x_{-1} = 2\langle \mathbf{x}, \mathbf{e}_0\rangle - \langle \mathbf{x}, \mathbf{e}_{-1}\rangle.
$$

Rearranging the terms

$$
x_0 = \frac{1}{2}\left[\langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta + \langle \mathbf{x}, \mathbf{e}_{-1}\rangle\right]
$$

establishing the base case. Now fix $n \le -1$ and suppose that for all $-1 \ge m \ge n$ we have

$$x_0 = \frac{|m|}{|m-1|}\langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta + \frac{|m+1|}{|m-1|}\langle \mathbf{x}, \mathbf{e}_{-1}\rangle_\Delta + \cdots + \frac{|-1|}{|m-1|}\langle \mathbf{x}, \mathbf{e}_{m+1}\rangle_\Delta + \frac{1}{|m-1|}\langle \mathbf{x}, \mathbf{e}_m\rangle.$$

By definition 2.2

$$\langle \mathbf{x}, \mathbf{e}_n\rangle_\Delta = -\langle \mathbf{x}, \mathbf{e}_{n+1}\rangle + 2\langle \mathbf{x}, \mathbf{e}_n\rangle - \langle \mathbf{x}, \mathbf{e}_{n-1}\rangle.$$

Rearranging the terms

$$x_n = \frac{1}{2}\left[\langle \mathbf{x}, \mathbf{e}_n\rangle_\Delta + \langle \mathbf{x}, \mathbf{e}_{n+1}\rangle + \langle \mathbf{x}, \mathbf{e}_{n-1}\rangle\right].$$

Substituting this into the above equation gives

$$\begin{aligned} x_0 &= \frac{|n|}{|n-1|}\langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta + \frac{|n+1|}{|n-1|}\langle \mathbf{x}, \mathbf{e}_{-1}\rangle_\Delta + \cdots + \frac{|-1|}{|n-1|}\langle \mathbf{x}, \mathbf{e}_{n+1}\rangle_\Delta \\ &+ \frac{1}{|n-1|}\frac{1}{2}\left[\langle \mathbf{x}, \mathbf{e}_n\rangle_\Delta + \langle \mathbf{x}, \mathbf{e}_{n+1}\rangle + \langle \mathbf{x}, \mathbf{e}_{n-1}\rangle\right]. \end{aligned}$$

Inductively we know

$$\langle \mathbf{x}, \mathbf{e}_{n+1}\rangle = |n|\langle \mathbf{x}, \mathbf{e}_0\rangle - |n+1|\langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta - |n+2|\langle \mathbf{x}, \mathbf{e}_{-1}\rangle_\Delta - \cdots - |-1|\langle \mathbf{x}, \mathbf{e}_{n+2}\rangle_\Delta.$$

Using this

$$\begin{aligned} \langle \mathbf{x}, \mathbf{e}_0\rangle &= \frac{|n|}{|n-1|}\langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta + \frac{|n+1|}{|n-1|}\langle \mathbf{x}, \mathbf{e}_{-1}\rangle_\Delta + \cdots + \frac{|-1|}{|n-1|}\langle \mathbf{x}, \mathbf{e}_{n+1}\rangle_\Delta \\ &+ \frac{1}{|n-1|}\frac{1}{2}\left[\langle \mathbf{x}, \mathbf{e}_n\rangle_\Delta + |n|\langle \mathbf{x}, \mathbf{e}_0\rangle - \sum_{j=0}^{|n+2|} |n+|j|+1|\langle \mathbf{x}, \mathbf{e}_j\rangle_\Delta + \langle \mathbf{x}, \mathbf{e}_{n-1}\rangle\right]. \end{aligned}$$

Collecting the terms

$$
\begin{aligned}
&\left[1-\frac{|n|}{2|n-1|}\right]\langle \mathbf{x},\mathbf{e}_0\rangle\\
&=\left[\left(|n|-\frac{|n+1|}{2}\right)\langle \mathbf{x},\mathbf{e}_0\rangle_\Delta+\left(|n+1|-\frac{|n+2|}{2}\right)\langle \mathbf{x},\mathbf{e}_{-1}\rangle_\Delta+\cdots+\left(2-\frac{1}{2}\right)\langle \mathbf{x},\mathbf{e}_{n+2}\rangle_\Delta\right.\\
&\left.+\langle \mathbf{x},\mathbf{e}_{n+1}\rangle_\Delta+\frac{1}{2}\langle \mathbf{x},\mathbf{e}_n\rangle_\Delta+\right]+\frac{1}{2|n-2|}\langle \mathbf{x},\mathbf{e}_{n-1}\rangle.
\end{aligned}
$$

Simplifying this

$$
\begin{aligned}
&\frac{|n-2|}{2|n-1|}\langle \mathbf{x},\mathbf{e}_0\rangle\\
&=\frac{1}{|n-1|}\left[\frac{|n-1|}{2}\langle \mathbf{x},\mathbf{e}_0\rangle_\Delta+\frac{|n|}{2}\langle \mathbf{x},\mathbf{e}_{-1}\rangle_\Delta+\cdots+\frac{3}{2}\langle \mathbf{x},\mathbf{e}_{n+2}\rangle_\Delta+\frac{2}{2}\langle \mathbf{x},\mathbf{e}_{n+1}\rangle_\Delta+\frac{1}{2}\langle \mathbf{x},\mathbf{e}_n\rangle_\Delta\right]\\
&+\frac{1}{2|n-1|}\langle \mathbf{x},\mathbf{e}_{n-1}\rangle,
\end{aligned}
$$

so that

$$
x_0=\frac{|n-1|}{|n-2|}\langle \mathbf{x},\mathbf{e}_0\rangle_\Delta+\frac{|n|}{|n-2|}\langle \mathbf{x},\mathbf{e}_{-1}\rangle_\Delta+\cdots+\frac{\langle \mathbf{x},\mathbf{e}_n\rangle_\Delta}{|n-2|}+\frac{\langle \mathbf{x},\mathbf{e}_{n-1}\rangle_\Delta}{|n-2|}
$$

completing the inductive step. Fix $\mathbf{x}\in H$ we have $\lim\limits_{\text{N}\to\text{-}\infty} x_N<\infty$. So in particular we have that $\lim\limits_{\text{N}\to\text{-}\infty}\frac{1}{|N-1|}\langle \mathbf{x},\mathbf{e}_N\rangle=0$. Thus setting $N=n+1$ we have

$$
\begin{aligned}
\langle \mathbf{x},\mathbf{e}_0\rangle&=\lim_{\text{N}\to\text{-}\infty}\frac{1}{|N-2|}\sum_{j=0}^{N}|N-j-1|\langle \mathbf{x},\mathbf{e}_j\rangle_\Delta+\lim_{\text{N}\to\text{-}\infty}\frac{1}{|N-2|}\langle \mathbf{x},\mathbf{e}_{N-1}\rangle_\Delta\\
&=\lim_{\text{N}\to\text{-}\infty}\frac{1}{|N-2|}\sum_{j=0}^{N}|N-j-1|\langle \mathbf{x},\mathbf{e}_j\rangle_\Delta.
\end{aligned}
$$

□

Now we convert from the basis $\{\mathbf{e}_m\}_{m=0}^{-\infty}$ to the basis $\{\hat{\mathbf{u}}_m\}_{m=0}^{-\infty}$.

Lemma 2.4. *For each $n\leq 0$*

$$\mathbf{e}_n = \sqrt{\frac{|n-2|}{|n-1|}}\hat{\mathbf{u}}_n - \sqrt{\frac{|n|}{|n-1|}}\hat{\mathbf{u}}_{n+1}. \tag{2.3}$$

Proof. Again we prove this by induction. The base case is automatic, since we have previously established that $\hat{\mathbf{u}}_0 = \frac{1}{\sqrt{2}}\mathbf{e}_0$. Now fix $n \leq 0$ and suppose that for all $0 \geq m \geq n$

$$\mathbf{e}_m = \sqrt{\frac{|m-2|}{|m-1|}}\hat{\mathbf{u}}_m - \sqrt{\frac{|m|}{|m-1|}}\hat{\mathbf{u}}_{m+1}.$$

Since

$$\hat{\mathbf{u}}_{n-1} = \frac{1}{\sqrt{|n-2||n-3|}}\left(\mathbf{e}_0 + \left(\sum_{j=-1}^{n}|j-1|\mathbf{e}_j\right) + |n-2|\mathbf{e}_{n-1}\right)$$

using the inductive hypothesis

$$\begin{aligned}
&\sqrt{|n-2||n-3|}\hat{\mathbf{u}}_{n-1} \\
&= \left(\sqrt{2}\hat{\mathbf{u}}_0 + \left(\sum_{j=-1}^{n}\sqrt{|j-1||j-2|}\hat{\mathbf{u}}_j - \sqrt{|j||j-1|}\hat{\mathbf{u}}_{j+1}\right) + |n-2|\mathbf{e}_{n-1}\right) \\
&= \sqrt{|n-1||n-2|}\hat{\mathbf{u}}_n + |n-2|\mathbf{e}_{n-1}.
\end{aligned}$$

Rearranging the terms again gives

$$\mathbf{e}_{n-1} = \frac{\sqrt{|n-2||n-3|}}{|n-2|}\hat{\mathbf{u}}_{n-1} - \frac{\sqrt{|n-1||n-2|}}{|n-2|}\hat{\mathbf{u}}_n = \sqrt{\frac{|n-3|}{|n-2|}}\hat{\mathbf{u}}_{n-1} - \sqrt{\frac{|n-1|}{n-2}}\hat{\mathbf{u}}_n$$

completing the induction. □

We can now use the above lemmas to compute the position of particle 0 in the $\hat{\mathbf{u}}_j$ basis.

Proposition 2.5. *The position of particle* 0*,* x_0*, is given by*

$$\lim_{\text{N}\to\text{-}\infty} \frac{1}{|N-2|}\left[\left(\frac{|N|}{\sqrt{2}}+\sqrt{2}\right)\langle \mathbf{x}, \hat{\mathbf{u}}_0\rangle_\Delta + \sum_{j=-1}^{N+1}\left(\frac{|N|}{\sqrt{|j-1||j-2|}}+2\sqrt{\frac{|j-1|}{|j-2|}}\right)\langle \mathbf{x}, \hat{\mathbf{u}}_j\rangle_\Delta\right] \tag{2.4}$$

Proof. The proof is just a calculation using the previous lemmas.

$$\begin{aligned}
&\lim_{\text{N}\to\text{-}\infty}\left[\frac{1}{|N-2|}\sum_{j=0}^{N}|N-j-1|\langle \mathbf{x}, \mathbf{e}_j\rangle_\Delta\right] \\
=&\lim_{\text{N}\to\text{-}\infty}\frac{1}{|N-2|}\Bigg[|N-1|\sqrt{2}\langle \mathbf{x}, \hat{\mathbf{u}}_0\rangle_\Delta \\
&+\sum_{j=-1}^{N}|N-j-1|\left(\sqrt{\frac{|j-2|}{|j-1|}}\langle \mathbf{x}, \hat{\mathbf{u}}_j\rangle_\Delta - \sqrt{\frac{|j|}{|j-1|}}\langle \mathbf{x}, \hat{\mathbf{u}}_{j+1}\rangle_\Delta\right)\Bigg] \\
=&\lim_{\text{N}\to\text{-}\infty}\frac{1}{|N-2|}\Bigg[|N-1|\sqrt{2}\langle \mathbf{x}, \hat{\mathbf{u}}_0\rangle_\Delta + \\
&\left(\sum_{j=-1}^{N}|N-j-1|\sqrt{\frac{|j-2|}{|j-1|}}\langle \mathbf{x}, \hat{\mathbf{u}}_j\rangle_\Delta\right. \\
&\left.-\left(\sum_{j=-2}^{N}|N-j-1|\sqrt{\frac{|j|}{|j-1|}}\langle \mathbf{x}, \hat{\mathbf{u}}_{j+1}\rangle_\Delta\right)\right) \\
&-|N-(-1)-1|\frac{1}{\sqrt{2}}\langle \mathbf{x}, \hat{\mathbf{u}}_0\rangle_\Delta\Bigg] \\
=&\lim_{\text{N}\to\text{-}\infty}\frac{1}{|N-2|}\Bigg[\left((|N|+1)\sqrt{2}-\frac{|N|}{\sqrt{2}}\right)\langle \mathbf{x}, \hat{\mathbf{u}}_0\rangle_\Delta \\
&+\sum_{j=-1}^{N+1}\left(|N-j-1|\sqrt{\frac{|j-2|}{|j-1|}}-|N-(j-1)-1|\sqrt{\frac{|j-1|}{|j-2|}}\right)\langle \mathbf{x}, \hat{\mathbf{u}}_j\rangle_\Delta \\
&+\sqrt{N-2}|N-1|\langle \mathbf{x}, \hat{\mathbf{u}}_n\rangle_\Delta\Bigg].
\end{aligned}$$

Since

$$\begin{aligned}
&(|N-j|+1)\sqrt{\frac{|j-2|}{|j-1|}}-\sqrt{\frac{|j-1|}{|j-2|}}|N-j| \\
=&|N-j|\left(\frac{|j-2|-|j-1|}{\sqrt{|j-2||j-1|}}\right)+\sqrt{\frac{|j-2|}{|j-1|}}
\end{aligned}$$

$$
\begin{aligned}
=&|N-j|\left(\frac{|j|+2-|j|-1}{\sqrt{|j-2||j-1|}}\right)+\sqrt{\frac{|j-2|}{|j-1|}}\\
=&\frac{|N-j|+|j-2|}{\sqrt{|j-2||j-1|}}=\frac{|N|}{\sqrt{|j-2||j-1|}}+2\sqrt{\frac{|j-1|}{|j-2|}}
\end{aligned}
$$

we can further simplify the previous string of equalities to get

$$
\begin{aligned}
\langle \mathbf{x}, \mathbf{e}_0\rangle = \lim_{\mathrm{N}\to\text{-}\infty} \frac{1}{|N-2|}\Bigg[&\left(|N|\left(\sqrt{2}-\frac{1}{\sqrt{2}}\right)+\sqrt{2}\right)\langle \mathbf{x}, \hat{\mathbf{u}}_0\rangle_\Delta\\
&+\sum_{j=-1}^{N+1}\left(\frac{|N|}{\sqrt{|j-1||j-2|}}+2\sqrt{\frac{|j-1|}{|j-2|}}\right)\langle \mathbf{x}, \hat{\mathbf{u}}_j\rangle_\Delta\\
&+\sqrt{\frac{|N-2|}{|N-1|}}\langle \mathbf{x}, \hat{\mathbf{u}}_N\rangle_\Delta.\Bigg]
\end{aligned}
$$

□

With $\langle \mathbf{x}, \mathbf{e}_0\rangle$ known we can determine expressions for the positions of every particle.

Lemma 2.6. *The position of particle $j-1$ is found recursively by*

$$
\begin{aligned}
\langle \mathbf{x}, \mathbf{e}_{-1}\rangle &= 2\langle \mathbf{x}, \mathbf{e}_0\rangle - \langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta\\
\langle \mathbf{x}, \mathbf{e}_{j-1}\rangle &= 2\langle \mathbf{x}, \mathbf{e}_j\rangle - \langle \mathbf{x}, \mathbf{e}_{j+1}\rangle - \langle \mathbf{x}, \mathbf{e}_j\rangle_\Delta
\end{aligned}
\tag{2.5}
$$

Proof. The proof is just application of the definition 2.2 on page 17. We simply observe that

$$\langle \mathbf{x}, \mathbf{e}_0\rangle_\Delta = 2\langle \mathbf{x}, \mathbf{e}_0\rangle - \langle \mathbf{x}, \mathbf{e}_{-1}\rangle$$

and

$$\langle \mathbf{x}, \mathbf{e}_j\rangle_\Delta = -\langle \mathbf{x}, \mathbf{e}_{j+1}\rangle + 2\langle \mathbf{x}, \mathbf{e}_j\rangle - \langle \mathbf{x}, \mathbf{e}_{k+1}\rangle$$

and rearrange the terms. □

We now want to understand the displacements of the particles as a random variable.

To do this we construct a probability probability space $(\Omega_q, \mathcal{B}, \mu_q)$ and a collection of i.i.d Gaussian random variables $\langle \mathbf{x}, \hat{\mathbf{u}}_i \rangle_\Delta$, $i \in \mathbb{Z}^-$ with mean zero and variance $k_B T/k^2$.

Existence of Ω_q turns out to be routine: we follow [11] to outline the construction. Let $\{\mu_k : k \in \mathbb{N}\}$ be a sequence of Gaussian, mean zero, variance $k_B T/k^2$ probability measures on $\mathbb{R}$ equipped with the Borel sigma algebra. The metric $d : \mathbb{R}^\infty \times \mathbb{R}^\infty \to \mathbb{R}$ given by

$$d(\mathbf{x}, \mathbf{y}) = \sum_{j \geq 1} 2^{-n} \frac{\max\{|x_k - y_k| : 1 \leq k \leq n\}}{1 + \max\{|x_k - y_k| : 1 \leq k \leq n\}},$$

turns $\mathbb{R}^\infty$ into a complete metric space with the same topology as the product topology on $\mathbb{R}^\infty$ [11]. One then defines the cylindrical subsets of $\mathbb{R}^\infty$ to be

$$I_{n,A} = \{\mathbf{x} \in \mathbb{R}^\infty : (x_1, \ldots, \mathbf{x}_n) \in A \subseteq \mathbb{R}^n\}.$$

The sigma algebra generated by the collection of cylindrical sets is precisely the Borel sigma algebra of $\mathbb{R}^\infty$. One then defines the function μ on the cylindrical sets by

$$\mu(I_{n,A}) == \mu_1 \times \cdots \times \mu_n(A),$$

where the μ_j are Lebesgue measures on $\mathbb{R}$. By the Caratheodory extension theorem, the function μ then extends uniquely to a probability measure on $\mathbb{R}^\infty$ [11]. The functional $\langle \cdot, q_j \rangle_\Delta : \mathbb{R}^\infty \to \overline{\mathbb{R}}$ has mean and variance

$$\int_{\mathbb{R}^\infty} \langle y, \mathbf{q}_j \rangle d\mu(y) = \int_{\mathbb{R}} y_k d\mu_k(y_k) = 0,$$

$$\int_{\mathbb{R}^\infty} \langle y, \mathbf{q}_j \rangle^2 d\mu(y) = \int_{\mathbb{R}} y_k^2 d\mu_k(y_k) = \frac{k_B T}{k^2},$$

where the $\{\mathbf{q}_j\}_{j=1}^\infty$ are the standard basis vectors in Ω_q. This proves the existence of a space with the *i.i.d* Gaussian random variables we desire. We now pushforward this measure onto H by the isomorphism $I : \Omega_q \to H$, $I(e_j) = \hat{u}_{-j+1}$. As an abuse of notation, we now identify the spaces Ω_q and H. The position of particle j is then the random variable corresponding to formulas 2.5 and 2.6 on pages 24 and 26 respectively, interpreted now as $L^2(\Omega_q)$ limits.

Lemma 2.7. *The position of particle* 0 *is a mean zero, variance* 1 *Gaussian random variable on* Ω_q.

Proof. We automatically have that $\langle \mathbf{x}, \mathbf{e}_0 \rangle$ is Gaussian. Thus it only remains to compute its mean and variance. The mean is automatically zero, since each $\langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta$ is mean zero. The variance is a similarly easy calculation. Since $\langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta$ are *i.i.d* mean zero variance one Gaussian random variables

$$
\begin{aligned}
&\mathrm{Var}\left[\langle \mathbf{x}, \mathbf{e}_0 \rangle\right] \\
=&\lim_{\mathrm{N}\to\text{-}\infty} \mathrm{Var}\left[\frac{1}{|N-2|}\left[\left(\frac{|N|}{\sqrt{2}}+\sqrt{2}\right)\langle \mathbf{x}, \hat{\mathbf{u}} \rangle_\Delta + \right.\right. \\
&\left.\left.\sum_{j=-1}^{N+1}\left(\frac{|N|}{\sqrt{|j-1||j-2|}}+2\sqrt{\frac{|j-1|}{|j-2|}}\right)\langle \mathbf{x}, \hat{\mathbf{u}}_0 \rangle_\Delta\right]\right] \\
=&\lim_{\mathrm{N}\to\text{-}\infty} \frac{1}{|N-2|^2}\left[\left(\frac{|N|}{\sqrt{2}}+\sqrt{2}\right)^2 + \right. \\
&\left.\left(\sum_{j=-1}^{N+1}\left(\frac{|N|}{\sqrt{|j-1||j-2|}}+2\sqrt{\frac{|j-1|}{|j-2|}}\right)^2\right)\right] \\
=&\lim_{\mathrm{N}\to\text{-}\infty} \frac{1}{|N-2|^2}\left[\frac{|N|^2}{2}+2|N|\right. \\
&\left.+2\left(\sum_{j=-1}^{N+1}\left(\frac{|N|^2}{|j-1||j-2|}+4\frac{|N|}{|j-2|}+4\frac{|j-1|}{|j-2|}\right)\right)\right] \\
=&\lim_{\mathrm{N}\to\text{-}\infty} \frac{1}{|N-2|^2}\left[\frac{|N|^2}{2}\left(\sum_{j=-1}^{N+1}\left(\frac{|N|^2}{|j-1||j-2|}+4\frac{|N|}{|j-2|}\right)\right)\right] \\
=&\frac{1}{2}+\lim_{\mathrm{N}\to\text{-}\infty}\frac{|N|^2}{|N-2|^2}\sum_{k=1}^{|N|-1}\frac{1}{(k+1)(k+2)}+\lim_{\mathrm{N}\to\text{-}\infty}\frac{|N|}{|N-2|^2}\sum_{k=1}^{|N|-1}\frac{1}{k+2}.
\end{aligned}
$$

However,

$$
\lim_{\mathrm{N}\to\text{-}\infty}\frac{|N|}{|N-2|^2}\sum_{k=1}^{|N|-1}\frac{1}{k+2}=0,
$$

giving

$$\mathrm{Var}\left[\langle \mathbf{x}, \mathbf{e}_0 \rangle\right] = \frac{1}{2} + \lim_{\text{N}\to\text{-}\infty} \frac{|N|^2}{|N-2|^2} \sum_{k=1}^{|N|-1} \frac{1}{(k+1)(k+2)} = \frac{1}{2} + \frac{1}{2} = 1,$$

proving the lemma. □

The main result of this section will be to determine the estimate of the variance of particle j. In order to do this, it will be useful to write the functional $\langle \mathbf{x}, \mathbf{e}_j \rangle$ in terms of the $\langle \mathbf{x}, \hat{\mathbf{u}}_i \rangle_\Delta$.

Lemma 2.8. *For $k \leq 0$, the position of the particle k is given by*

$$\langle \mathbf{x}, \mathbf{e}_k \rangle = \lim_{\text{N}\to\text{-}\infty} \frac{|k-1|}{|N-2|} \left[\sum_{j=k}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \right]. \tag{2.6}$$

Proof. The proof is given by induction. By inspection for the formula given for $\langle \mathbf{x}, \mathbf{e}_0 \rangle$ in lemma 2.7 automatically satisfies this formula. I will instead choose to start the induction at $k = -1$ for convenience. For the base case,

$$\begin{aligned}
&\langle \mathbf{x}, \mathbf{e}_{-1} \rangle = 2\langle \mathbf{x}, \mathbf{e}_0 \rangle - \langle \mathbf{x}, \mathbf{e}_0 \rangle_\Delta \\
=&2 \lim_{\text{N}\to\text{-}\infty} \frac{1}{|N-2|} \left[\left(\frac{|N|}{\sqrt{2}} + \sqrt{2} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_0 \rangle_\Delta \right. \\
&\left. + \sum_{j=-1}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \right] \\
&- \langle \mathbf{x}, \sqrt{2}\hat{\mathbf{u}}_0 \rangle_\Delta \\
=& \lim_{\text{N}\to\text{-}\infty} \frac{2}{|N-2|} \left[\left(\frac{|N|}{\sqrt{2}} + \sqrt{2} - \frac{|N-2|}{2}\sqrt{2} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_0 \rangle_\Delta \right. \\
&\left. + \sum_{j=-1}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \right].
\end{aligned}$$

Simplifying the first term

$$
\begin{aligned}
&\frac{|N|}{\sqrt{2}} + \sqrt{2} - \frac{\sqrt{2}|N-2|}{2} = \frac{\sqrt{2}|N| - \sqrt{2}|N-2|}{2} + \sqrt{2} \\
&= \frac{\sqrt{2}\left[|N| - |N-2|\right]}{2} + \sqrt{2} = \frac{\sqrt{2}}{2}\left[|N| - |N| - 2\right] + \sqrt{2} = 0,
\end{aligned}
$$

and so

$$
\langle \mathbf{x}, \mathbf{e}_{-1} \rangle = \lim_{\text{N}\to\text{-}\infty} \frac{2}{|N-2|} \left[\sum_{j=-1}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \right],
$$

establishing the base case. Now assume that for all $-1 \geq l \geq k$

$$
\begin{aligned}
&\langle \mathbf{x}, \mathbf{e}_l \rangle \\
&= \lim_{\text{N}\to\text{-}\infty} \frac{|l-1|}{|N-2|} \left[\sum_{j=l}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \right. \\
&\left. + \sqrt{\frac{|N-2|}{|N-1|}} \langle \mathbf{x}, \hat{\mathbf{u}}_N \rangle_\Delta \right].
\end{aligned}
$$

Again from lemma 2.6

$$
\langle \mathbf{x}, \mathbf{e}_{k-1} \rangle = 2\langle \mathbf{x}, \mathbf{e}_k \rangle - \langle \mathbf{x}, \mathbf{e}_{k+1} \rangle - \langle \mathbf{x}, \mathbf{e}_k \rangle_\Delta.
$$

Using the inductive hypothesis

$$
\begin{aligned}
&\langle \mathbf{x}, \mathbf{e}_{k-1} \rangle \\
&= \lim_{\text{N}\to\text{-}\infty} \frac{|k-1|}{|N-2|} \left[\sum_{j=k}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \right] \\
&- \lim_{\text{N}\to\text{-}\infty} \frac{|k|}{|N-2|} \left[\sum_{j=k+1}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \right] \\
&- \left\langle \mathbf{x}, \sqrt{\frac{|k-2|}{|k-1|}} \hat{\mathbf{u}}_k - \sqrt{\frac{|k|}{|k-1|}} \hat{\mathbf{u}}_{k+1} \right\rangle_\Delta
\end{aligned}
$$

$$= \lim_{\text{N}\to\text{-}\infty} \frac{1}{|N-2|} \Bigg[\left(-|k| \left(\frac{|N|}{\sqrt{|k||k-1|}} + 2\sqrt{\frac{|k|}{|k-1|}} \right) + \sqrt{\frac{|k|}{|k-1|}}|N-2| \right) \langle \mathbf{x}, \hat{\mathbf{u}}_{k+1} \rangle_\Delta$$

$$\left(2|k-1| \left(\frac{|N|}{\sqrt{|k-1||k-2|}} + 2\sqrt{\frac{|k-1|}{|k-2|}} \right) - |k| \left(\frac{|N|}{\sqrt{|k-1||k-2|}} + 2\sqrt{\frac{|k-1|}{|k-2|}} \right) \right.$$

$$\left. -|N-2|\sqrt{\frac{|k-2|}{|k-1|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_k \rangle_\Delta$$

$$+ (2|k-1| - |k|) \sum_{j=k-1}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \Bigg].$$

Thankfully,

$$- |k| \left(\frac{|N|}{\sqrt{|k||k-1|} + 2\sqrt{\frac{|k|}{|k-1|}}} \right) + |N-2|\sqrt{\frac{|k|}{|k-1|}}$$
$$= (|N-2| - |N|) \sqrt{\frac{|k|}{|k-1|}} - 2\sqrt{\frac{|k|}{|k-1|}} = 2\sqrt{\frac{|k|}{|k-1|}} - 2\sqrt{\frac{|k|}{|k-1|}} = 0$$

eliminating the first term. The second term will vanish as well, but the calculation is slightly more involved:

$$\begin{aligned}
&2|k-1| \left(\frac{|N|}{\sqrt{|k-1||k-2|}} + 2\sqrt{\frac{|k-1|}{|k-2|}} \right) \\
&\quad - |k| \left(\frac{|N|}{\sqrt{|k-1||k-2|}} + 2\sqrt{\frac{|k-1|}{|k-2|}} \right) - |N-2|\sqrt{\frac{|k-2|}{|k-1|}} \\
=&(2|k-1| - |k|) \left(\frac{|N|}{\sqrt{|k-1||k-2|}} + 2\sqrt{\frac{|k-1|}{|k-2|}} \right) - |N-2|\sqrt{\frac{|k-2|}{|k-1|}} \\
=&(|k|+2) \left(\frac{|N|}{\sqrt{|k-1||k-2|}} + 2\sqrt{\frac{|k-1|}{|k-2|}} \right) - |N-2|\sqrt{\frac{|k-2|}{|k-1|}} \\
=&|k-2| \left(\frac{|N|}{\sqrt{|k-1||k-2|}} + 2\sqrt{\frac{|k-1|}{|k-2|}} \right) - |N-2|\sqrt{\frac{|k-2|}{|k-1|}} \\
=&|N|\sqrt{\frac{|k-2|}{|k-1|}} + 2\sqrt{|k-1||k-2|} - |N-2|\sqrt{\frac{|k-2|}{|k-1|}}
\end{aligned}$$

$$=(|N|-|N|-2)\sqrt{\frac{|k-2|}{|k-1|}}+2\sqrt{|k-1||k-2|}$$
$$=-2\sqrt{\frac{|k-2|}{|k-1|}}+2\sqrt{|k-1||k-2|}.$$

Since this term is independent of N,

$$\lim_{\text{N}\to\text{-}\infty}\frac{1}{|N-2|}\left[-2\sqrt{\frac{|k-2|}{|k-1|}}+2\sqrt{|k-1||k-2|}\right]\langle\mathbf{x},\hat{\mathbf{u}}_k\rangle_\Delta=0,$$

and since $|k-2|=(2|k-1|-|k|)$, we conclude

$$\langle\mathbf{x},\mathbf{e}_{k-1}\rangle=\lim_{\text{N}\to\text{-}\infty}\frac{|k-2|}{|N-2|}\left[\sum_{j=k-1}^{N+1}\left(\frac{|N|}{\sqrt{|j-1||j-2|}}+2\sqrt{\frac{|j-1|}{|j-2|}}\right)\langle\mathbf{x},\hat{\mathbf{u}}_j\rangle_\Delta\right],$$

completing the inductive step. □

Theorem 2.9. *For $k\leq 0$, the position of particle k is a mean zero variance variance $|k-1|$ Gaussian random variable on Ω_q.*

Proof. Lemma 2.7 already establishes the result for the zeroth particle, and lemma 2.8 shows that $\langle\mathbf{x},\mathbf{e}_k\rangle$ is always a limit of sums of Gaussian mean zero random variables on Ω_q, so that it itself is a Gaussian mean zero random variable on Ω_q. It remains only to compute the variance of $\langle\mathbf{x},\mathbf{e}_k\rangle$ for $k\leq -1$. Calculating,

$$\begin{aligned}&\operatorname{Var}(\langle\mathbf{x},\mathbf{e}_k\rangle)\\&=\lim_{\text{N}\to\text{-}\infty}\frac{|k-1|^2}{|N-2|^2}\left[\sum_{j=k}^{N+1}\left(\frac{|N|}{\sqrt{|j-1||j-2|}}+2\sqrt{\frac{|j-1|}{|j-2|}}\right)^2+\frac{|N-2|}{|N-1|}\right]\\&=\lim_{\text{N}\to\text{-}\infty}\frac{|k-1|^2}{|N-2|^2}\sum_{j=k}^{N+1}\left(\frac{|N|}{\sqrt{|j-1||j-2|}}+2\sqrt{\frac{|j-1|}{|j-2|}}\right)^2\\&=\lim_{\text{N}\to\text{-}\infty}\frac{|k-1|^2}{|N-2|^2}\sum_{j=k}^{N+1}\left(\frac{|N|^2}{|j-1||j-2|}+4\frac{|N|}{|j-2|}+\frac{|j-1|}{|j-2|}\right)\end{aligned}$$

$$
\begin{aligned}
&= \lim_{\text{N}\to\text{-}\infty} \frac{|k-1|^2}{|N-2|^2} \sum_{j=k}^{N+1} \frac{|N|^2}{|j-1||j-2|} \\
&=|k-1|^2 \lim_{\text{N}\to\text{-}\infty} \sum_{j=|k|}^{|N|-1} \frac{1}{(j+1)(j+2)} \\
&=|k-1|^2 \left[\sum_{j=1}^{\infty} \frac{1}{(j+1)(j+2)} - \sum_{j=1}^{|k|-1} \frac{1}{(j+1)(j+2)} \right] \\
&=|k-1|^2 \left[\frac{1}{2} - \sum_{j=1}^{|k|-1} \frac{1}{(j+1)(j+2)} \right] \\
&=|k-1|^2 \left[\frac{1}{2} - \sum_{j=1}^{|k|-1} \left(\frac{1}{j+1} - \frac{1}{j+2} \right) \right] \\
&=|k-1|^2 \left[\frac{1}{2} - \left(\frac{1}{2} - \frac{1}{|k|-1+2} \right) \right] \\
&=|k-1|^2 \left[\frac{1}{|k|+1} \right] \\
&=|k-1|^2 \frac{1}{|k-1|} \\
&=|k-1|,
\end{aligned}
$$

proving the theorem. $\square$

Lemma 2.8 also lets us compute the covariances of the positions.

Theorem 2.10. *For $k, l \leq 0$, the covariance of $\langle \mathbf{x}, \mathbf{e}_j \rangle$ and $\langle \mathbf{x}, \mathbf{e}_l \rangle$ is $|\max(j, l) - 1|$.*

Proof. The proof is almost identical to the above. Without loss of generality, fix $k \leq l \leq 0$. Since $\langle \mathbf{x}, \mathbf{e}_j \rangle$ is a mean zero random variable,

$$
\begin{aligned}
&\mathrm{Cov}(\langle \mathbf{x}, \mathbf{e}_k \rangle, \langle \mathbf{x}, \mathbf{e}_l \rangle) = \int_{\Omega_q} \langle \mathbf{x}, \mathbf{e}_k \rangle \langle \mathbf{x}, \mathbf{e}_l \rangle d\mu_q \\
&= \int_{\Omega_q} \lim_{M,N\to-\infty} \frac{|k-1|}{|N-2|} \left[\sum_{j=k}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_j \rangle_\Delta \right] \\
&\frac{|l-1|}{|M-2|} \left[\sum_{j'=l}^{M+1} \left(\frac{|M|}{\sqrt{|j'-1||j'-2|}} + 2\sqrt{\frac{|j'-1|}{|j'-2|}} \right) \langle \mathbf{x}, \hat{\mathbf{u}}_{j'} \rangle_\Delta \right] d\mu_q.
\end{aligned}
$$

Since we have already established the $L^2(\Omega_q)$ convergence of $\langle \mathbf{x}, \mathbf{e}_k \rangle$, by Cauchy-Scwartz and dominated convergence (the integral is dominated by the product of the variances of $\langle x, \mathbf{e}_j \rangle, \langle x, \mathbf{e}_l \rangle$ allow the limits to be pulled outside the integral. The covariance then becomes

$$\mathrm{Cov}(\langle \mathbf{x}, \mathbf{e}_k \rangle, \langle \mathbf{x}, \mathbf{e}_l \rangle) \quad = \lim_{N \to -\infty} \frac{|k-1||l-1|}{|N-2|^2} \sum_{j=k}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right)^2 .$$

Following the calculation of theorem 2.9

$$\begin{aligned} &= \lim_{N \to -\infty} \frac{|k-1||l-1|}{|N-2|^2} \sum_{j=k}^{N+1} \left(\frac{|N|}{\sqrt{|j-1||j-2|}} + 2\sqrt{\frac{|j-1|}{|j-2|}} \right)^2 \\ &= \lim_{\text{N} \to \text{-}\infty} |k-1||l-1| \frac{1}{|k-1|} = |k-1| = |\max(k,l) - 1|. \end{aligned}$$

$\square$

2.2 Equilibrium Invariance of Observables

In this section it is shown that the algebra of observables generated by the displacements and momenta are invariant under the flow of the measure on phase space.

Similar to the previous construction, the Caratheodory extension theorem establishes the existence of the probability space where $(\Omega_p, \mu_p) = \bigotimes_{i \le 0} (\mathbb{R}, \mu_i)$ where each μ_i is a mean zero Gaussian measure on R with variance $k_B T / k^2$. As done previously, to simplify notation I will be assuming $k_B T = k^2$ for the remained of the section.

Definition 2.5. *Let $h^{-2p} \subset \mathbb{R}^{\mathbb{Z}^-}$ be the Hilbert space of sequences with norm*

$$|| \, \mathbf{x} \, ||_{h^{-2p}}^2 = \sum_{j \le 0} \frac{x_j^2}{(1 + |j|^2)^p}. \tag{2.7}$$

Definition 2.6. *Define $\mathcal{L} : h^{-2p} \to h^{-2p}$ by*

$$-\mathcal{L}\mathbf{e}_0 = -2\mathbf{e}_0 + \mathbf{e}_{-1}, \quad -\mathcal{L}\mathbf{e}_j = \mathbf{e}_{j-1} - 2\mathbf{e}_j + \mathbf{e}_{j+1},\, j \leq -1. \tag{2.8}$$

Lemma 2.11. *The operator $\mathcal{L}$ is bounded on h^{-2p}.*

Proof. Fix $\mathbf{x} \in h^{-2p}$. Then,

$$\begin{aligned}
||\mathcal{L}\,\mathbf{x}||^2_{h^{-2p}} &= \left|\left| -2x_0\mathbf{e}_0 + x_0\mathbf{e}_{-1} + \sum_{n\leq -1} x_n\mathbf{e}_{n-1} - 2x_n\mathbf{e}_n + x_n\mathbf{e}_{n+1} \right|\right|^2_{h^{-2p}} \\
&= \left|\left| \lim_{\text{N}\to\text{-}\infty} (-2x_0 + x_1)\mathbf{e}_0 + \sum_{n=-1}^{N} (x_{n-1} - 2x_n + x_{n+1})\mathbf{e}_j + x_{N+1}\mathbf{e}_N \right|\right|^2_{h^{-2p}} \\
&= (-2x_0 + x_1)^2 + \sum_{n=-1}^{N} \frac{(x_{n-1} - 2x_n + x_{n+1})^2}{(1+|n|^2)^p} + \frac{x_{N+1}^2}{(1+|N|^2)^p} \\
&= (-2x_0 + x_1)^2 + \sum_{n=-1}^{N} \frac{(x_{n-1} - 2x_n + x_{n+1})^2}{(1+|n|^2)^p} \qquad \big((\text{ since } \mathbf{x} \in h^{-2p}\big) \\
&\leq C\left[x_0^2 + x_{-1}^2 + \sum_{n\leq -1} \frac{x_{n-1}^2 + x_n^2 + x_{n+1}^2}{(1+|n|^2)^p} \right] \\
&\leq C\left[3||\,\mathbf{x}\,||_{||\,\mathbf{x}\,||_{h^{-2p}}} + \sum_{n\leq -1} \frac{x_{n-1}^2}{(1+|n|^2)^p} + \sum_{n\leq -1} \frac{x_{n+1}^2}{(1+|n|^2)^p} \right] \\
&\leq C\left[||\,\mathbf{x}\,||_{h^{-2p}} + \sum_{n\leq -2} \frac{x_n^2}{(1+|n+1|^2)^p} + \sum_{n\leq 0} \frac{x_n^2}{(1+|n-1|^2)^p} \right] \\
&\leq C\left[||\,\mathbf{x}\,||_{h^{-2p}} + \sum_{n\leq -2} \frac{x_n^2}{(1+|n+1|^2)^p} + ||\,\mathbf{x}\,||_{h^{-2p}} \right] \\
&\leq C\left[||\,\mathbf{x}\,||_{h^{-2p}} + \sum_{n\leq -2} \frac{2x_n^2}{(1+|n|^2)^p} \right] \quad \left(\text{using } \frac{1}{1+|j+1|^2} \leq \frac{2}{1+|j|^2} \text{ for all } j \right) \\
&\leq C||\,\mathbf{x}\,||_{h^{-2p}},
\end{aligned}$$

where the constant C varies line from line, but is independent of $\mathbf{x}$. □

Lemma 2.12. *The operator $\mathcal{L}$ is positive definite on h^{-2p}.*

Proof. Using the convention that $x_j = 0$ for $j > 0$ we see

$$
\begin{aligned}
\langle \mathcal{L}\,\mathbf{x}, \mathbf{x}\rangle_{h^{-2p}} &= \sum_{j,k\leq 0} x_j x_k \left(\langle -e_{j-1} + 2e_j - e_{j+1}, e_k\rangle_{h^{-2p}}\right) \\
&= \sum_{j\leq 0} x_j \left(-\frac{x_{j-1}}{(1+|j-1|^2)^p} + 2\frac{x_j}{(1+|j|^2)^p} - \frac{x_{j+1}}{(1+|j+1|^2)^p}\right) \\
&= x_0^2 + \sum_{j\leq 0}\left(\frac{x_j}{(1+|j|^2)^p} - \frac{x_{j-1}}{(1+|j-1|^2)^p}\right)^2 \geq 0.
\end{aligned}
$$

Moreover if $\langle \mathcal{L}\,\mathbf{x}, \mathbf{x}\rangle_{h^{-2p}} = 0$, then $x_0 = 0$ and $x_j = x_{j-1}$ for all $j \leq 0$ finishing the proof. □

Definition 2.7. *Let H^{-2p} be the Banach space defined by the norm $||\,\mathbf{x}\,||^2_{H^{-2p}} := ||\sqrt{\mathcal{L}}\,\mathbf{x}\,||^2_{h^{-2p}}$.*

Definition 2.8. *Let $B_p = h^{-2p} \times H^{-2p}$ be the product Banach space with norm $||(\mathbf{p}, \mathbf{q})^T||_B = ||\,\mathbf{p}\,||_{h^{-2p}} + ||\,\mathbf{q}\,||_{H^{-2p}}$.*

Definition 2.9. *Let $(\Omega = \Omega_p \times \Omega_q, d\mu_p \otimes d\mu_q)$ be the Banach space with norm $||(\mathbf{p}, \mathbf{q})^T||^2_\Omega = \mathbb{E}\left[||(\mathbf{p}, \mathbf{q})^T||^2_B\right]$.*

Lemma 2.13. *Fix $p > 1$, then $||\,\mathbf{x}\,||^2_\Omega = \mathbb{E}\left[||(\mathbf{p}, \mathbf{q})^T||^2_B\right] < \infty$.*

Proof. By the monotone convergence theorem, boundedness of $\mathcal{L}$, and theorem 2.10:

$$
\begin{aligned}
||(\mathbf{p}, \mathbf{q})^T||^2_\Omega &= \mathbb{E}\left[||(\mathbf{p}, \mathbf{q})^T||^2_{B_p}\right] \\
&= \int_\Omega ||\,\mathbf{p}\,||^2_{h^{-2p}} + ||\,\mathbf{q}\,||^2_{H^{-2p}} d\mu_p d\mu_q \\
&= \int_\Omega \sum_{j\leq 0} \frac{p_j^2}{(1+|j|^2)^p} d\mu_p d\mu_q + \int_\Omega ||\sqrt{\mathcal{L}} q||^2_{h^{-2p}} d\mu_p d\mu_q \\
&\leq C\left[\sum_{j\leq 0} \frac{1}{(1+|j|^2)^p} \int_{\mathbb{R}} p_j^2 d\mu_{p_j} + \int_\Omega ||q||^2_{h^{-2p}} d\mu_p d\mu_q\right] \\
&= C\left[\sum_{j\leq 0} \frac{1}{(1+|j|^2)^p} + \int_\Omega \frac{q_j^2}{(1+|j|^2)^p} d\mu_p d\mu_q\right]
\end{aligned}
$$

$$
\begin{aligned}
&= C\left[\sum_{j\le 0}\left(\frac{1}{(1+|j|^2)^p} + \frac{1}{(1+|j|^2)^p}\int_{\mathbb{R}} q_j^2 d\mu_{q_j}\right)\right] \\
&= C\left[\sum_{j\le 0}\left(\frac{1}{(1+|j|^2)^p} + \frac{|j-1|}{(1+|j|^2)^p}\right)\right] < \infty,
\end{aligned}
$$

for some constant $C > 0$ since $p > 1$. □

For the remainder of the section we will assume $p > 1$ is fixed.

Definition 2.10. *Let A be the linear operator defined on the Banach space Ω be given by $A(\mathbf{p}, \mathbf{q})^T = (\mathcal{L}\,\mathbf{q}, \mathbf{p})^T$.*

Lemma 2.14. *The operator A is bounded on Ω.*

Proof. Using the boundedness of $\mathcal{L}$ and the definition of the norm of H^{-2p} we find

$$
\begin{aligned}
&\mathbb{E}\left[||A(\mathbf{p}, \mathbf{q})^T||_{B_p}^2\right] = \mathbb{E}\left[||\mathcal{L}\,\mathbf{q}\,||_{h^{-2p}}^2 + ||\,\mathbf{p}\,||_{H^{-2p}}^2\right] \\
&\le C\,\mathbb{E}\left[||\sqrt{\mathcal{L}}\,\mathbf{q}\,||_{h^{-2p}}^2 + ||\sqrt{\mathcal{L}}\,\mathbf{p}\,||_{h^{-2p}}^2\right] \\
&\le C\mathbb{E}\left[||\,\mathbf{q}\,||_{H^{-2p}}^2 + ||\,\mathbf{p}\,||_{h^{-2p}}^2\right] \\
&= C\mathbb{E}\left[||(\mathbf{p}, \mathbf{q})^T||_{B_p}^2\right].
\end{aligned}
$$

□

Lemma 2.15. *The second order ODE system $\ddot{\mathbf{q}}(t) = \mathcal{L}\,\mathbf{q}(t)$ with initial conditions $(\mathbf{p}, \mathbf{q})^T \in \Omega$ has global in time solution given by $(\mathbf{p}(t), \mathbf{q}(t))^T = e^{tA}(\mathbf{p}, \mathbf{q})^T$.*

Proof. When written as a first order system we see that $\frac{d}{dt}(\mathbf{p}(t), \mathbf{q}(t))^T = A(\mathbf{p}(t), \mathbf{q}(t))^T$ with $\dot{\mathbf{q}} = \mathbf{p}$. Since A is a bounded operator e^{tA} exists for all t completing the proof. □

For notational convenience in the sequel, let p_j denote the functional $\langle -, e_{p_j}\rangle$ and similarly for q_j unless otherwise stated.

Definition 2.11. *Let Ω' be the continuous dual space of the Banach space Ω.*

Definition 2.12. *Let $\mathcal{O} = \overline{Alg\{p_j, q_j : j \leq 0\}}$ be closure of the Algebra generated by all the functionals p_j, q_j $j \leq 0$ in the norm topology on Ω'.*

Theorem 2.16. *For every $f \in \mathcal{O}$ we have that $\mathbb{E}[f] = \mathbb{E}\left[f \circ e^{tA}\right]$.*

Proof. Since every $f \in \mathcal{O}$ is an infinite sum of products of Gaussian random variables we have that $\mathbb{E}[f]$ is a sum of products of $\mathbb{E}[p_j], \mathbb{E}[q_j], \mathbb{E}[p_j p_k], \mathbb{E}[p_j q_k]$, and $\mathbb{E}[q_j q_k]$. Since $\mathbb{E}[p_j] = \mathbb{E}[q_j] = 0$ it suffices to check that $\mathbb{E}[p_j p_k] = \mathbb{E}[p_j p_k \circ e^t A], \mathbb{E}[p_j q_k] = \mathbb{E}\left[p_j q_k \circ e^{tA}\right]$, and $\mathbb{E}[q_j q_k] = \mathbb{E}\left[q_j q_k \circ e^{tA}\right]$. Choose any two $e_1, e_2 \in \{p_j, q_j : j \leq 0\}$. Then note that,

$$
\begin{aligned}
&\frac{d}{dt}\mathbb{E}\left[e_1 e_2 \circ e^{tA}\right] \\
&= \frac{d}{dt}\int_\Omega \langle e_1, e^{tA}(\mathbf{p},\mathbf{q})^T\rangle\langle e_2, e^{tA}(\mathbf{p},\mathbf{q})^T\rangle d\mu_p d\mu_q \quad (e_1, e_2 \text{ the corresponding vectors }) \\
&= \frac{d}{dt}\int_\Omega e_1 \otimes e_2 \left[e^{tA} \otimes e^{tA}\left((\mathbf{p},\mathbf{q})^T \otimes (\mathbf{p},\mathbf{q})^T\right)\right] d\mu_p d\mu_q \\
&= \int_\Omega e_1 \otimes e_2 \left[e^{tA} \otimes e^{tA}\left(A(\mathbf{p},\mathbf{q})^T \otimes (\mathbf{p},\mathbf{q})^T + (\mathbf{p},\mathbf{q})^T \otimes A(\mathbf{p},\mathbf{q})^T\right)\right] d\mu_p d\mu_q \\
&= e_1 \otimes e_2 \left[e^{tA} \otimes e^{tA}\left(\int_\Omega A(\mathbf{p},\mathbf{q})^T \otimes (\mathbf{p},\mathbf{q})^T + (\mathbf{p},\mathbf{q})^T \otimes A(\mathbf{p},\mathbf{q})^T d\mu_p d\mu_q\right)\right].
\end{aligned}
$$

However note that,

$$
\begin{aligned}
&\int_\Omega A(\mathbf{p},\mathbf{q})^T \otimes (\mathbf{p},\mathbf{q})^T + (\mathbf{p},\mathbf{q})^T \otimes A(\mathbf{p},\mathbf{q})^T d\mu_p d\mu_q \\
&= \int_\Omega \begin{pmatrix} \mathcal{L}\,\mathbf{q}\otimes\mathbf{p} + \mathcal{L}\,\mathbf{p}\otimes\mathbf{q} & \mathbf{p}\otimes\mathbf{p} + L\,\mathbf{q}\otimes\mathbf{q} \\ \mathbf{p}\otimes\mathbf{p} + \mathcal{L}\,\mathbf{q}\otimes\mathbf{q} & \mathbf{p}\otimes\mathbf{q} + \mathbf{q}\otimes\mathbf{p} \end{pmatrix} d\mu_p d\mu_q.
\end{aligned}
$$

To evaluate this integral note that the diagonal blocks are automatically zero since

$$
\int_\Omega p_i q_j d\mu_p d\mu_q = 0.
$$

For the off diagonal elements using theorem 2.10 on page 33,

$$\int_{\Omega} (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q = \delta_{jk} + \left[-\mathbb{E}\left[q_j q_{k+1}\right] + \mathbb{E}\left[q_j q_k\right] - \mathbb{E}\left[q_j q_{k-1}\right]\right].$$

We continue in cases: Case 1: $k < 0$, and $j < k - 1$

$$\begin{aligned}
&\int_{\Omega} (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q \\
&= 0 + [|\max(j, k-1) - 1| - 2|\max(j, k) - 1| + |\max(j, k+1) - 1|] \\
&= [|k-2| - 2|k-1| + |k|] \\
&= |k| + 2 - 2|k| - 2 + |k| = 0.
\end{aligned}$$

Case 2: $k < 0$, and $j > k + 1$

$$\begin{aligned}
&\int_{\Omega} (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q \\
&= 0 + [|\max(j, k-1) - 1| - 2|\max(j, k) - 1| + |\max(j, k+1) - 1|] \\
&= [|j-1| - 2|j-1| + |j-1|] = 0.
\end{aligned}$$

Case 3: $k < 0$, and $j = k - 1$

$$\begin{aligned}
&\int_{\Omega} (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q \\
&= 0 + [|\max(j, k-1) - 1| - 2|\max(j, k) - 1| + |\max(j, k+1) - 1|] \\
&= |k-2| - 2|k-1| + |k| \\
&= |k| + 2 - 2|k| - 2|k| = 0.
\end{aligned}$$

Case 4: $k < 0$, and $j = k$

$$\begin{aligned}
&\int_{\Omega} (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q \\
&= 1 + [|\max(j, k-1) - 1| - 2|\max(j, k) - 1| + |\max(j, k+1) - 1|]
\end{aligned}$$

$$= 1 + |k-1| - 2|k-1| + |k|$$
$$= 1 + |k| + 1 - 2|k| - 2 + |k| = 0.$$

Case 5: $k < 0$, and $j = k + 1$

$$\int_\Omega (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q$$
$$= 0 + [|\max(j, k-1) - 1| - 2|\max(j,k) - 1| + |\max(j, k+1) - 1|]$$
$$= |k| - 2|k| + |k| = 0.$$

Case 6: $k = 0$ $j \leq -2$

$$\int_\Omega (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q$$
$$= 0 + [|\max(j, k-1) - 1| - 2|\max(j,k) - 1|]$$
$$= |-2| - 2|-1| = 0.$$

Case 7: $k = 0$ $j = -1$

$$\int_\Omega (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q$$
$$= 0 + [|\max(j, k-1) - 1| - 2|\max(j,k) - 1|]$$
$$= |-2| - 2|-1| = 0.$$

Case 8: $k = 0$ $j = 0$

$$\int_\Omega (p_j p_k - q_j \mathcal{L} q_k) d\mu_p d\mu_q$$
$$= 1 + [|\max(j, k-1) - 1| - 2|\max(j,k) - 1|]$$
$$= 1 + |-1| - 2|-1| = 0.$$

Combining all the above cases we can conclude that

$$\int_{\Omega} \begin{pmatrix} \mathcal{L}\,\mathbf{q}\otimes\mathbf{p}+\mathcal{L}\,\mathbf{p}\otimes\mathbf{q} & \mathbf{p}\otimes\mathbf{p}+L\,\mathbf{q}\otimes\mathbf{q} \\ \mathbf{p}\otimes\mathbf{p}+\mathcal{L}\,\mathbf{q}\otimes\mathbf{q} & \mathbf{p}\otimes\mathbf{q}+\mathbf{q}\otimes\mathbf{p} \end{pmatrix} d\mu_p d\mu_q = 0,$$

and so by linearity

$$\frac{d}{dt}\mathbb{E}\left[e_1 e_2 \circ e^{tA}\right] = 0,$$

completing the proof. $\square$

Chapter 3

Deriving the Green's Functions

3.1 Hilbert Space of Initial Displacements

Definition 3.1. *Let* $\langle\cdot,\cdot\rangle_\Delta : \mathbb{R}^{\mathbb{Z}} \times \mathbb{R}^{\mathbb{Z}} \to \overline{\mathbb{R}}$ *be given by*

$$\begin{aligned}&\langle \mathbf{x}, \mathbf{y}\rangle_\Delta \\ &= \lim_{\mathrm{N}\to\infty} \left\langle \sum_{i=-N+1}^{N-1} \left(-x_{i+1} + 2x_i - x_{i-1}\right) \mathbf{e}_i, +(2x_N - x_{N-1})\mathbf{e}_N + (2x_{-N} - x_{-N+1})\mathbf{e}_{-N}, \right. \\ &\qquad \left. \sum_{i=-N}^{N} y_i \mathbf{e}_i \right\rangle.\end{aligned}$$

Proposition 3.1. *The function* $\langle\cdot,\cdot\rangle_\Delta$ *is an inner product on the space*

$$\tilde{H} = \{\mathbf{x} \in \mathbb{R}^{\mathbb{Z}} : \langle \mathbf{x}, \mathbf{x}\rangle_\Delta < \infty\}.$$

Proof. By construction $\langle\cdot,\cdot\rangle_\Delta$ is bilinear and well-defined, so it suffices to check symmetry and positive definiteness. First we check symmetry:

$$\langle \mathbf{x}, \mathbf{y}\rangle = \lim_{\mathrm{N}\to\infty} \sum_{i=-N+1}^{N-1} (-x_{i+1} + 2x_i - x_{i-1}) y_i + (2x_N - x_{N-1}) y_N + (2x_{-N} - x_{-N+1}) y_{-N}$$

$$
\begin{aligned}
&= \lim_{\mathrm{N}\to\infty} \left[\sum_{i=-N+1}^{-1} (-x_{i+1} + 2x_i - x_{i-1})y_i + (-x_{-1} + 2x_0 - x_1)y_0 \right. \\
&+ \sum_{i=1}^{N-1} (-x_{i+1} + 2x_i - x_{i-1})y_i \\
&\left. +(2x_N - x_{N-1})y_N + (2x_{-N} - x_{-N+1})y_{-N} \right] \\
&= \lim_{\mathrm{N}\to\infty} \left[(x_0 - x_{-1})y_0 \sum_{i=-N+1}^{-1} (-x_{i+1} + 2x_i - x_{i-1})y_i + (2x_{-N} - x_{-N+1})y_{-N} \right. \\
&\left. +(x_0 - x_1)y_0 + \sum_{i=1}^{N-1} (-x_{i+1} + 2x_i - x_{i-1})y_i(2x_N - x_{N-1})y_N \right] \\
&= \lim_{\mathrm{N}\to\infty} \left[x_0(y_0 - y_{-1}) + \sum_{j=2}^{N} x_{-j+1}(-y_{-j+2} + 2y_{-j+1} - y_{-j})x_{-j+1} \right. \\
&+x_{-N}(2y_{-N} - y_{-N+1}) \\
&\left. +x_0(y_0 - y_1) + \sum_{j=2}^{N} x_{j-1}(-y_{j-2} + 2y_{j-1} - y_j) + x_N(2y_N - y_{N-1}) \right] \\
&= \langle \mathbf{y}, \mathbf{x} \rangle_\Delta.
\end{aligned}
$$

As for positive definiteness,

$$
\begin{aligned}
&\langle \mathbf{x}, \mathbf{x} \rangle_\Delta \\
&= \lim_{\mathrm{N}\to\infty} \left[\sum_{k=-N+1}^{N-1} (-x_{k+1} + 2x_k - x_{k-1})x_k + (2x_N - x_{N-1})x_N + (2x_{-N} - x_{-N+1})x_{-N} \right] \\
&= \lim_{\mathrm{N}\to\infty} \left[(x_0 - x_{-1})x_0 + \sum_{k=-N+1}^{-1} (-x_{k+1} + 2x_k - x_{k-1})x_k + (2x_{-N} - x_{-N+1})x_{-N} \right. \\
&\quad \left. +(x_0 - x_1)x_0 + \sum_{k=1}^{N-1} (-x_{k+1} + 2x_k - x_{k-1})x_k + (2x_N - x_{N-1})x_N \right] \\
&= \lim_{\mathrm{N}\to\infty} \left[\sum_{k=-N+1}^{0} (x_k - x_{k-1})^2 + x_{-N}^2 + \sum_{k=0}^{N-1} (x_k - x_{k+1})^2 + x_N^2 \right] \geq 0.
\end{aligned}
$$

Moreover when $\langle x, x \rangle_\Delta = 0$ we have that $x_k = x_k + 1$ for all $k \in \mathbb{Z}$ and that $\lim_{\mathrm{N}\to\infty} x_k = 0$, showing that $x_k = 0$ for all k, and thus $\mathbf{x} = 0$, completing the proof. □

Definition 3.2. *Let $(H, \langle , \rangle_\Delta)$ be the smallest by inclusion Hilbert space containing $(\tilde{H}, \langle , \rangle_\Delta)$.*

Definition 3.3. *Further let $||\cdot||_\Delta$ be the norm induced by the inner product on H.*

The set $\{\mathbf{e}_j : j \in \mathbb{Z}\}$ is not a basis for H, for if we suppose that $\mathbf{x} \in H$ with $\langle \mathbf{x}, \mathbf{e}_j \rangle_\Delta = 0$ for all $j \in \mathbb{Z}$, then we have the infinite set of finite difference equations $-x_{j-1} + 2x_j - x_{j+1} = 0$ for each $j \in \mathbb{Z}$. However the vector of all 1's, denoted $\mathbb{1} = \sum_{j\in\mathbb{Z}} \mathbf{e}_j \in H$, satisfies $\langle \mathbb{1}, \mathbf{e}_j \rangle_\Delta = 0$ for all $j \in \mathbb{Z}$, but clearly $\mathbb{1} \neq 0$. It will turn out to be somewhat more mathematically convenient to have a dual representation for $\mathbb{1}$.

Definition 3.4. *Let $l : H \to \mathbb{R}$ be given by $l(\mathbf{x}) := \langle \mathbf{x}, \mathbb{1} \rangle_\Delta := \langle \mathbf{x}, \mathbf{e}_\infty \rangle_\Delta$.*

Proposition 3.2. *The set $\{\mathbf{e}_j\}_{j\in\mathbb{Z}} \cup \{\mathbf{e}_\infty\}$ is a basis for H.*

Proof. Fix $\mathbf{x} \in H$ and suppose that $\langle \mathbf{x}, \mathbf{e}_j \rangle_\Delta = 0$ for all j and that $\langle \mathbf{x}, \mathbf{e}_\infty \rangle_\Delta = 0$. This gives

$$-x_{j-1} + 2x_j - x_{j+1} = 0 \text{ for all } j \in \mathbb{Z}, \text{ and } \lim_{\mathrm{N}\to\infty} x_N = 0.$$

It turns out that these relations imply the following: For all $n \geq 1$, $-x_{-1} + \frac{n+1}{n} f_0 - \frac{x_n}{n} = 0$. We proceed by induction. The base case is automatic since

$$\langle \mathbf{x}, \mathbf{e}_0 \rangle_\Delta = -x_{-1} + \frac{1+1}{2} x_0 - \frac{x_1}{1} = 0.$$

Now fix $n > 1$ and assume that for all j, $1 \leq j \leq n$ that

$$-x_{-1} + \frac{j+1}{j} x_0 - \frac{x_j}{j} = 0.$$

Since we have assumed

$$\langle \mathbf{x}, \mathbf{e}_n \rangle_\Delta = -x_{n-1} + 2x_n - x_{n+1} = 0,$$

we may rearrange this equality to obtain

$$x_n = \frac{x_{n-1} + x_{n+1}}{2}.$$

Substituting this into the inductive hypothesis for $j = n$ gives

$$-x_{-1}+\frac{n+1}{n}x_0-\frac{x_n}{n}=-x_{-1}+\frac{n+1}{n}x_0-\frac{\frac{x_{n-1}+x_{n+1}}{2}}{n}=0.$$

However, the inductive hypothesis for $j=n-1$ also gives that

$$-(n-1)x_{-1}+nx_0=x_{n-1},$$

and so we can conclude

$$-x_{-1}+\frac{n+1}{n}x_0-\frac{(-(n-1)x_{-1}+nx_0)}{2n}-\frac{x_{n+1}}{2n}=0.$$

Rearranging the terms,

$$\left(\frac{n-1}{2n}-1\right)x_{-1}+\left(\frac{n+1}{n}-\frac{1}{2}\right)x_0-\frac{x_{n+1}}{2n}=0$$

$$\left(\frac{n-1-2n}{2n}\right)x_{-1}+\left(\frac{2n+2-n}{2n}\right)x_0-\frac{x_{n+1}}{2n}=0$$

$$\frac{-(n+1)}{2n}x_{-1}+\frac{n+2}{2n}x_0-\frac{x_{n+1}}{2n}=0$$

$$-(n+1)x_{-1}+(n+2)x_0-f_{n+1}=0$$

$$-x_{-1}+\frac{n+2}{n+1}x_0-\frac{f_{n+1}}{n+1}=0,$$

completing the inductive step and establishing that for all $n\geq 1$, $-x_{-1}+\frac{n+1}{n}f_0-\frac{x_n}{n}=0$. Passing to the limit as $n\to\infty$ then gives

$$\lim_{\mathrm{N}\to\infty}-x_{-1}+\frac{N+1}{N}x_0-\frac{x_N}{N}=-f_{-1}+f_0=0,$$

as $\mathbf{x}\in H$ automatically implies $\lim_{\mathrm{N}\to\infty}\frac{x_N}{N}=0$. In particular this tells us that $x_0=x_{-1}$, and that the result of the claim reduces to

$$-x_0+\frac{n+1}{n}x_0-\frac{x_n}{n}=0,$$

for all $n \geq 1$. Simplifying this gives that

$$\left(\frac{n+1}{n} - 1\right) x_0 - \frac{x_n}{n} = 0$$

$$\frac{1}{n} x_0 = \frac{1}{n} x_n$$

$$x_0 = x_n$$

for all $n \geq 1$. Since we already established that $x_0 = x_{-1}$, we have that for all $n \geq -1$, $x_n = x_0$.

The positivity of n in the above arguments was purely superficial analogous statements hold for negative n. I will now show this with the following claim. For $j \leq -1$,

$$-x_1 + \frac{|j|+1}{|j|} x_0 - \frac{x_j}{|j|} = 0.$$

Again we prove this by induction. Since $\langle \mathbf{x}, \mathbf{e}_0 \rangle_\Delta = 0$, we have that

$$-x_1 + \frac{|-1|+1}{|-1|} x_0 - \frac{x_{-1}}{|-1|} = 0$$

establishing the base case. Now fix $n < -1$ and assume for all j, $n \leq j \leq -1$ we have that

$$-x_1 + \frac{|j|+1}{|j|} x_0 - \frac{x_j}{|j|} = 0.$$

Since $-x_{n-1} + 2x_n - x_{n+1} = 0$, we can solve for x_n and substitute the result into the inductive hypothesis on n:

$$-x_1 + \frac{|n|+1}{|n|} x_0 - \frac{x_{n-1} + x_{n+1}}{2|n|} = 0.$$

However, by the inductive hypothesis

$$-x_1 + \frac{|n+1|+1}{|n+1|} x_0 - \frac{x_{n+1}}{|n+1|} = -x_1 + \frac{|n|}{|n|-1} x_0 - \frac{x_{n+1}}{|n|-1} = 0.$$

Substituting this into the previous equation then gives

$$
\begin{aligned}
&-x_1 + \frac{|n|+1}{|n|}x_0 - \frac{-(|n|-1)x_1 + |n|x_0}{2|n|} - \frac{x_{n-1}}{2|n|} = 0 \\
&\left(\frac{|n|-1}{2|n|} - 1\right)x_1 + \left(\frac{|n|+1}{|n|} - \frac{1}{2}\right)x_0 - \frac{x_{n-1}}{2|n|} = 0 \\
&\left(\frac{-|n|-1}{2|n|}\right)x_1 + \left(\frac{|n|+2}{2|n|}\right)x_0 - \frac{x_{n-1}}{2|n|} = 0 \\
&-(|n|+1)x_1 + (|n|+2)x_0 - x_{n-1} = 0 \\
&-x_1 + \frac{|n|+2}{|n|+1}x_0 - \frac{x_{n-1}}{|n|+1} = 0 \\
&-x_1 + \frac{|n-1|+1}{|n-1|}x_0 - \frac{x_{n-1}}{|n-1|} = 0,
\end{aligned}
$$

completing the inductive step. So for each $n \leq -1$

$$-x_1 + \frac{|n|+1}{|n|}x_0 - \frac{x_n}{|n|} = 0,$$

but we already established that $x_1 = x_0$, and so we can quickly see that $x_n = x_0$ for all $n \in \mathbb{Z}$. Now using the assumption that $\langle x, \mathbf{e}_i nfty\rangle = 0$, we get that $x_n = 0$, for all $n \in \mathbb{Z}$ completing the proof. $\square$

At this point we will want to define our discrete Laplace operator $\mathcal{L} : H \to H$, however to do so we need to make a decision one how $\mathcal{L}$ will act on $\mathbf{e}_\infty$. A natural choice is to make whatever choice which makes $\mathcal{L}$ a self-adjoint operator. The only such is $\mathcal{L}\mathbf{e}_\infty = 0$.

Definition 3.5. *Let $\mathcal{L} : H \to H$ be the linear operator defined by*

$$\mathcal{L}\mathbf{e}_i = k^2(-\mathbf{e}_{i-1} + 2\mathbf{e}_i - \mathbf{e}_{i+1}), \quad \mathcal{L}\mathbf{e}_\infty = 0. \tag{3.1}$$

In order to carry through with our spectral representation of $\mathcal{L}$ on H, we will need to show $\mathcal{L}$ is self adjoint.

Proposition 3.3. *The operator $\mathcal{L}$ is a bounded symmetric operator on H.*

Proof. First some notation. For convenience of notation set $k^2 = 1$. For any $y \in H$, let $(\mathbf{y})_i = y_i = \langle \mathbf{y}, \mathbf{e}_i \rangle$. Now fix $\mathbf{x} \in H$. Then we know

$$||\mathcal{L}\,\mathbf{x}\,||^2_\Delta = \lim_{\mathrm{N}\to\text{-}\infty} (\mathcal{L}\,\mathbf{x})^2_N + \sum_{i=-\infty}^{0} ((\mathcal{L}\,\mathbf{x})_i - (\mathcal{L}\,\mathbf{x})_{i-1})^2 + \sum_{i=0}^{\infty} ((\mathcal{L}\,\mathbf{x})_i - (\mathcal{L}\,\mathbf{x})_{i+1})^2 + \lim_{\mathrm{N}\to\infty} (\mathcal{L}\,\mathbf{x})^2_N.$$

However, a simple calculation shows that

$$\lim_{N\to\pm\infty} (\mathcal{L}\,\mathbf{x})^2_N = \left(\lim_{N\to\pm\infty} -x_{N-1} + 2x_N - x_{N+1} \right)^2 = 0,$$

and so the norm, $||\mathcal{L}\,\mathbf{x}\,||^2_\Delta$ simplifies to

$$\begin{aligned}
&||\mathcal{L}\,\mathbf{x}\,||^2_\Delta \\
=& \sum_{i=-\infty}^{0} ((\mathcal{L}\,\mathbf{x})_i - (\mathcal{L}\,\mathbf{x})_{i-1})^2 \\
&\quad + \sum_{i=0}^{\infty} ((\mathcal{L}\,\mathbf{x})_i - (\mathcal{L}\,\mathbf{x})_{i+1})^2 \\
=& \sum_{i=-\infty}^{0} (-x_{i-1} + 2x_i - x_{i+1} + x_{i-2} - 2x_{i-1} + x_i)^2 \\
&\quad + \sum_{i=0}^{\infty} (-x_{i-1} + 2x_i - x_{i+1} + x_i - 2x_{i+1} + 2x_{i+2})^2 \\
=& \sum_{i=-\infty}^{0} ((x_{i-2} - x_{i-1}) + 2(x_i - x_{i-1}) + (x_i - x_{i+1}))^2 \\
&\quad + \sum_{i=0}^{\infty} ((x_i - x_{i-1}) + (x_{i+2} - x_{i+1}) + 2(x_i - x_{i+1}))^2 \\
\leq& \sum_{i=-\infty}^{0} \left[(x_{i-2} - x_{i-1})^2 + 4(x_i - x_{i-1})^2 + (x_i - x_{i+1})^2 \right] \\
&+ \sum_{i=0}^{\infty} \left[(x_i - x_{i-1})^2 + 4(x_i - x_{i+1})^2 + (x_{i+2} - x_{i+1})^2 \right] \\
=& (x_0 - x_{-1})^2 + \sum_{i=0}^{\infty} (x_i - x_{i+1})^2 + \sum_{i=1}^{\infty} (x_i - x_{i+1})^2 + 4\sum_{i=0}^{\infty} (x_i - x_{i+1})^2
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{i=-\infty}^{-1}(x_i-x_{i-1})^2+4\sum_{i=-\infty}^{0}(x_i-x_{i-1})^2+(x_0-x_1)^2+\sum_{i=-\infty}^{0}(x_i-x_{i-1})^2\\
\leq&\sum_{i=-\infty}^{0}(x_i-x_{i-1})^2+\sum_{i=0}^{\infty}(x_i-x_{i+1})^2+\lim_{\text{N}\to\text{-}\infty}x_N^2+\lim_{\text{N}\to\infty}x_N^2\\
&+\sum_{i=0}^{\infty}(x_i-x_{i+1})^2+\sum_{i=-\infty}^{0}(x_i-x_{i-1})^2+\lim_{\text{N}\to\text{-}\infty}x_N^2+\lim_{\text{N}\to\infty}x_N^2\\
&+4\left[\sum_{i=0}^{\infty}(x_i-x_{i+1})^2+\sum_{i=-\infty}^{0}(x_i-x_{i-1})^2+\lim_{\text{N}\to\text{-}\infty}x_N^2+\lim_{\text{N}\to\infty}x_N^2\right]\\
\leq&7||\,\mathbf{x}\,||_\Delta^2,
\end{aligned}
$$

proving boundedness of $\mathcal{L}$ on H. Fix $\mathbf{y}\in H$. It suffices to check that $\langle \mathcal{L}\mathbf{e}_\infty,\mathbf{y}\rangle_\Delta = \langle \mathbf{e}_\infty,\mathcal{L}\,\mathbf{y}\rangle_\Delta$ and for each $j\in\mathbb{Z}$, $\langle \mathcal{L}\mathbf{e}_j,\mathbf{y}\rangle_\Delta=\langle \mathbf{e}_j,\mathcal{L}\,\mathbf{y}\rangle_\Delta$. By definition

$$\langle \mathcal{L}\mathbf{e}_\infty,\mathbf{y}\rangle_\Delta=\langle 0,\mathbf{y}\rangle_\Delta=0.$$

Calculating we find

$$\langle \mathbf{e}_\infty,\mathcal{L}y\rangle_\Delta=\lim_{\text{N}\to\infty}(y_{N-1}+2y_N-y_{N+1})=0,$$

establishing $\langle \mathcal{L}\mathbf{e}_\infty,\mathbf{y}\rangle_\Delta=\langle \mathbf{e}_\infty,\mathcal{L}\,\mathbf{y}\rangle_\Delta$. Now fix $j\in\mathbb{Z}$. Then

$$
\begin{aligned}
\langle \mathcal{L}\mathbf{e}_j,\mathbf{y}\rangle_\Delta=&\langle -\mathbf{e}_{j-1}+2\mathbf{e}_j-\mathbf{e}_{j+1},\mathbf{y}\rangle_\Delta\\
=&-(-y_{j-2}+2y_{j-1}-y_j)+2(-y_{j-1}+2y_j-y_{j+1})-(-y_j+2y_j-y_{j+2})\\
=&y_{j-2}-2y_{j-1}+y_j-2y_{j-1}+4y_j-2y_{j+1}+y_j-2y_{j+1}+y_{j+2}\\
=&y_{j-2}-4y_{j-1}+6y_j-4y_{j+1}+y_{j+2},
\end{aligned}
$$

and

$$
\begin{aligned}
\langle \mathbf{e}_j,\mathcal{L}y\rangle_\Delta=&\langle \mathcal{L}y,\mathbf{e}_j\rangle_\Delta\\
=&\left\langle \sum_{k=-\infty}^{\infty}(-y_{k-1}+2y_k-y_{k+1})\mathbf{e}_k,\mathbf{e}_j\right\rangle_\Delta\\
=&-(-y_{j-2}+2y_{j-1}-y_j)+2(-y_{j-1}+2y_j-y_{j+1})-(y_j+2y_{j+1}-y_{j+2})\\
=&y_{j-2}-4y_{j-1}+6y_j-4y_{j+1}+y_{j+2},
\end{aligned}
$$

establishing $\langle \mathcal{L}\mathbf{e}_j, \mathbf{y}\rangle_\Delta = \langle \mathbf{e}_j, \mathcal{L}\,\mathbf{y}\rangle_\Delta$, and thus proving that $\mathcal{L}$ is a self adjoint operator. $\square$

Now that we have established that $\mathcal{L}$ is a self adjoint operator on H, we want to find a unitary representation of H which diagonalizes $\mathcal{L}$. Since all of the preceeding formalism is in an effort to have a spectral representation of $\mathcal{L}$ on H so that we can write down explicit solutions to our Green's functions, we may use that the initial data of the Green's functions however lives in a very particular subspace of H. In particular, we need only understand $\mathcal{L}$ restricted to this subspace in order to proceed with the analysis.

Definition 3.6. *Let* $W = \left\{ x \in H : \lim_{\mathrm{N}\to\infty} x_N = 0,\ \lim_{\mathrm{N}\to-\infty} x_N = 0 \right\}$.

Proposition 3.4. *The subspace W is closed.*

Proof. W is clearly a subspace of H. It is closed since the functional $x \mapsto \lim_{\mathrm{N}\to\infty} x_N^2 + \lim_{\mathrm{N}\to-\infty} x_N^2$ is automatically continuous in the $||\cdot||_\Delta$ norm, and W is the preimage of 0 by construction. $\square$

Proposition 3.5. *The operator L satisfies $\mathcal{L}(H) \subseteq W$.*

Proof. Let $\mathbf{x} \in H$. Then

$$\lim_{N\to\pm\infty} \langle \mathcal{L}\,\mathbf{x}, \mathbf{e}_N\rangle = \lim_{N\to\pm\infty} k^2(-x_{N-1} + 2x_N - x_{N+1}) = 0,$$

so $\mathcal{L}\,\mathbf{x} \in W$. $\square$

Definition 3.7. *The map $L : W \to W$ is given by $L := \mathcal{L}|_W$.*

Definition 3.8. *Let μ be the measure on $[0, 2\pi]$ with Radon-Nikodym derivative given by* $\frac{d\mu}{dx} = 2(1 - \cos(x))$, *where dx is the Lebesgue measure.*

Definition 3.9. *Define the weighted L^2 space by* $L^2([0, 2\pi], d\mu) = \left\{ f : [0, 2\pi] \to \mathbb{C} : \int_0^{2\pi} |f(x)|^2 d\mu_x < \right.$

Definition 3.10. *Let $U : W \to L^2([0, 2\pi], d\mu)$ be given by*

$$U(\mathbf{a}) = U\left(\sum_{j=-\infty}^{\infty} \langle \mathbf{a}, \mathbf{e}_j\rangle e_j\right) = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} \langle \mathbf{a}, \mathbf{e}_j\rangle e^{ijx}. \tag{3.2}$$

In order to verify that the codomain of U is in fact $L^2([0,2\pi],d\mu)$, we must compute $||U(a)||^2_{L^2(d\mu)}$ for arbitrary $a \in W$.

Lemma 3.6. *For all* $\mathbf{a} \in W$, $||U(\mathbf{a})||^2_{L^2(d\mu)} = ||\mathbf{a}||^2_\Delta$.

Proof. Fix $\mathbf{a} \in L^2(d\mu)$. Then

$$
\begin{aligned}
&||U(\mathbf{a})||^2_{L^2(d\mu)} \\
=&\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}\sum_{j=-\infty}^{\infty} a_j e^{ijx}\overline{U(a)}2(1-\cos(x))dx \\
=&\frac{1}{\sqrt{2\pi}}\sum_{j=-\infty}^{\infty} a_j \int_0^{2\pi} e^{ijx}\sum_{k=-\infty}^{\infty}\frac{a_k}{\sqrt{2\pi}}e^{-ikx}2(1-\cos(x))dx \\
=&\frac{1}{2\pi}\sum_{j=-\infty}^{\infty} a_j \int_0^{2\pi}\sum_{k=-\infty}^{\infty} a_k\left(-e^{i((j+1)-k)x}+2e^{i(j-k)x}-e^{i((j-1)-k)x}\right)dx \\
=&\frac{1}{2\pi}\sum_{j=-\infty}^{\infty} a_j \lim_{\mathrm{N}\to\infty}\int_0^{2\pi}\Bigg(\left[\sum_{k=-N}^{N}(-a_{k-1}+2a_k-a_{k+1})e^{i(j-k)x}\right] \\
&\quad +a_{-N-1}e^{i(j+N)x}+a_{N+1}e^{i(j-N)x}\Bigg)dx \\
=&\sum_{j,k=-\infty}^{\infty} a_j(-a_{k-1}+2a_k-a_{k+1})\delta_{kj}+\sum_{j=-\infty}^{\infty} a_j\lim_{\mathrm{N}\to\infty} a_{-N-1}\delta_{j,-N} \\
&\quad +\sum_{j=-\infty}^{\infty} a_j\lim_{\mathrm{N}\to\infty} a_{N+1}\delta_{jN} \\
=&\sum_{j=-\infty}^{\infty} a_j(-a_{j-1}+2a_j-a_{j+1}) \\
=&||\mathbf{a}||^2_\Delta,
\end{aligned}
$$

where the limit being pulled out is justified by Plancherel's theorem. □

Lemma 3.6 establishes U is a norm preserving map and that $L^2([0,2\pi],d\mu)$ is the appropriate codomain. From here we will want to show that U is unitary, and explicitly compute the adjoint of U.

Proposition 3.7. *The operator* U *has adjoint* $U^*: L^2([0,2\pi],d\mu)\to W$ *given by*

$$(U^*f)_n = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} f(x) e^{-inx} dx. \tag{3.3}$$

Proof. Let $f \in L^2([0, 2\pi], d\mu)$. Computing the adjoint we find

$$\begin{aligned}
&\langle U^* f, \mathbf{a} \rangle_\Delta \\
=&\langle f, U(\mathbf{a}) \rangle_{L^2(d\mu)} \\
=&\frac{1}{\sqrt{2\pi}} \int_0^{2\pi} f(x) \sum_{j=-\infty}^{\infty} a_j e^{-ijx} 2(1 - \cos x) dx \\
=&\frac{1}{\sqrt{2\pi}} \int_0^{2\pi} f(x) \sum_{j=-\infty}^{\infty} a_j \left(-e^{-i(j+1)x} + 2e^{-ijx} - e^{-i(j-1)x} \right) dx \\
=&\frac{1}{\sqrt{2\pi}} \lim_{\mathrm{N} \to \infty} \int_0^{2\pi} f(x) \left[\sum_{j=-N}^{N} (-a_{j-1} + 2a_a - a_{j+1}) e^{-ijx} + a_{-N-1} e^{iNx} + a_{N+1} e^{-iNx} \right] dx \\
=&\frac{1}{\sqrt{2\pi}} \lim_{\mathrm{N} \to \infty} \left[\sum_{j=-N}^{N} (-a_{j-1} + 2a_j - a_{j+1}) \int_0^{2\pi} f(x) e^{-ijx} dx \right] \\
=&\langle \mathbf{a}, \mathbf{f} \rangle_\Delta ,
\end{aligned}$$

where by definition $(\mathbf{f})_N = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} f(x) e^{-iNx} dx$. Going from the third to fourth line requires the following estimate:

$$\left| \int_0^{2\pi} f(x) e^{iNx} dx \right| = \left| \left\langle f(x), \frac{e^{iNx}}{2(1 - \cos x)} \right\rangle_{L^2(d\mu)} \right| \le ||f||_{L^2(d\mu)} \left|\left| \frac{e^{iNx}}{2(1 - \cos x)} \right|\right|_{L^2(d\mu)}$$

$$\le ||f||_{L^2(d\mu)} ||e^{iNx}||_{L^2(dx)} \lesssim ||f||_{L^2(d\mu)}.$$

Thus the adjoint is defined by $U^* f = \mathbf{f}$. □

Proposition 3.8. *The map U is a unitary.*

Proof. It suffices to show that $UU^* = I_{L^2([0,2\pi],d\mu)}$ and that $U^*U = I_W$. These proofs are essentially the same as the inversion proofs in Fourier analysis.

$$
\begin{aligned}
UU^*(f)(x) = U &\left(\frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} \int_0^{2\pi} f(y) e^{-ijy} dy \mathbf{e}_j \right) \\
=&\frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \left(\int_0^{2\pi} f(y) e^{-iky} dy \right) e^{ikx} \\
=&\frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \left(\int_0^{2\pi} f(y) e^{-ik(y-x)} dy \right) \\
=&\int_0^{2\pi} f(y) \delta(y-x) dy \\
=&f(x).
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
U^*U(\mathbf{a}) =&U^* \left(\frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} a_j e^{ijx} \right) \\
=&\frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \int_0^{2\pi} \left(\sum_{j=-\infty}^{\infty} a_j e^{ijx} \right) e^{-ikx} dx \mathbf{e}_k \\
=&\frac{1}{2\pi} \sum_{k,j=-\infty}^{\infty} a_j \int_0^{2\pi} e^{i(j-k)x} dx \mathbf{e}_k \\
=&\sum_{k,j=-\infty}^{\infty} a_j \delta_{jk} \mathbf{e}_k \\
=&\mathbf{a}.
\end{aligned}
$$

□

Definition 3.11. *Let $\hat{L} : L^2([0, 2\pi], d\mu) \to L^2([0, 2\pi], d\mu)$ be defined by*

$$
\hat{L} = ULU^* \tag{3.4}
$$

Proposition 3.9. *The spectrum of L is $[0, 4k^2]$.*

Proof. By proposition 3.8, it follows that $\sigma_W(L) = \sigma_{L^2([0,2\pi],d\mu)}\left(\hat{L}\right)$, where σ denotes the spectrum of the operator. Let $f \in L^2([0, 2\pi], d\mu)$. Then

$$
\begin{aligned}
\left(\hat{L}f\right)(y) &= \left(UL\sum_{k\in\mathbb{Z}}\left[\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} f(x)e^{-ikx}dx\right]\mathbf{e}_k\right)(y)\\
&= \left(U\sum_{k\in\mathbb{Z}}\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} f(x)e^{-ikx}k^2\left[-\mathbf{e}_{k+1}+2\mathbf{e}_k-\mathbf{e}_{k-1}\right]dx\right)(y)\\
&= k^2\left(U\sum_{k\in\mathbb{Z}}\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} f(x)\left[-e^{-i(k-1)x}+2e^{-ikx}-e^{-i(k+1)x}\right]\mathbf{e}_k dx\right)(y)\\
&= k^2\left(U\sum_{k\in\mathbb{Z}}\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} f(x)e^{-ikx}2(1-\cos(x))dx\right)(y)\\
&= \frac{1}{\sqrt{2\pi}}\sum_{k\in\mathbb{Z}}\left(\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} f(x)\left[2(1-\cos(x))\right]e^{-ikx}dx\right)e^{iky}\\
&= k^2\frac{1}{2\pi}\sum_{k\in\mathbb{Z}}\int_0^{2\pi} f(x)\left[2(1-\cos(x))\right]e^{-ik(x-y)}dx\\
&= 2k^2(1-\cos(y))f(y),
\end{aligned}
$$

showing that $\hat{L}$ has no eigenvalues. Now we need to figure out what values are in the resolvent of $\hat{L}$ exists. We know that L is self adjoint since it is the restriction of a self-adjoint operator to a closed subspace. This tells us that the spectrum of $\hat{L}$ is a subset of $\mathbb{R}$.

Fix $f \in L^2([0,2\pi], d\mu)$, $\lambda \notin [0, 4k^2]$ and define $g(x)$ by

$$g(x) = \frac{f(x)}{2k^2(1-\cos x)-\lambda}.$$

Since $\lambda \notin [0, 4k^2]$ there exists $c > 0$ such that $\left|\frac{1}{2k^2(1-\cos(x))-\lambda}\right| < c$, and so

$$||g||_{L^2(d\mu)} \lesssim ||f||_{L^2(d\mu)},$$

showing that $g \in L^2([0,2\pi], d\mu)$. But by construction,

$$\left(\hat{L}-\lambda I\right)(g)(x) = (2k^2(1\cos x)-\lambda)g(x) = f(x),$$

so we see that $\lambda \notin \sigma\left(\hat{L}\right)$.

Now let $\lambda \in [0,4]$. Since $\frac{1}{\sqrt{2k^2(1-\cos(x))}} \in L^2([0,2\pi], d\mu)$, but

$$\frac{1}{[2k^2(1-\cos x)-\lambda]\sqrt{2k^2(1-\cos x)}}$$

satisfies

$$\begin{aligned}\left\|\frac{1}{[2k^2(1-\cos x)-\lambda]\sqrt{2k^2(1-\cos x)}}\right\|_{L^2(d\mu)}\\ = \left\|\frac{1}{2k^2(1-\cos x)-\lambda}\right\|_{L^2(dx)} = \infty,\end{aligned}$$

and so $\dfrac{1}{[2k^2(1-\cos x)-\lambda]\sqrt{2k^2(1-\cos x)}}$ is not in $L^2([0,2\pi], d\mu)$. This shows that $(\hat{L}-\lambda I)$ cannot be surjective for $\lambda \in [0,4k^2]$. Hence we find that $\sigma(L) = \sigma\left(\hat{L}\right) = [0,4k^2]$. $\square$

The spectral theorem now allows us to write down how L, and certain functions of L, act on vectors in W [48]. Using the spectral theorem and what we have previously described above, if $h \in L^2([0,2\pi], d\mu)$, and $f : \mathbb{C} \to \mathbb{C}$ is entire (or any borel function),

$$(U^*(Uf(L)U^*h))_j = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} f\left(2k^2(1-\cos x)\right) h(x) e^{-ijx}dx.$$

However, for any $h \in L^2([0,2\pi], d\mu)$ there exists $\mathbf{h} \in W$ with $\mathbf{h} = Uh$. In particular we may represent any $h(x) = \dfrac{1}{\sqrt{2\pi}}\displaystyle\sum_{k\in\mathbb{Z}} h_k e^{ikx}$ for some $\mathbf{h} \in W$, where h_k is the k-th component of $\mathbf{h}$. This establishes the following theorem.

Theorem 3.10. *For any* $\mathbf{h} \in W$ *and* $f : \mathbb{C} \to \mathbb{C}$ *entire,*

$$f(L)\mathbf{h} = \sum_{j\in\mathbb{Z}} \frac{1}{2\pi}\left(\int_0^{2\pi} f(2k^2(1-\cos x)) \sum_{l\in\mathbb{Z}} e^{i(l-j)x} h_l \mathbf{e}_j dx\right). \tag{3.5}$$

Proof. The preceding argument. $\square$

3.2 Solving for the Green's Functions

From definition 1.20 on page 12, it is easy to see that the Green's functions have an operator form solution given by $\mathbf{g}_M(t) = \frac{\sin t\sqrt{L}}{\sqrt{L}}\,\mathbf{g}'_M(0)$.

Lemma 3.11. *The Green's function* $\mathbf{g}_M(t)$ *satisfies*

$$\mathbf{g}_M(t) = \frac{1}{\sqrt{2\pi}} \sum_{j\in\mathbb{Z}} \int_0^{2\pi} \frac{\sin\left(tk\sqrt{2(1-\cos x)}\right)}{k\sqrt{2(1-\cos x)}} e^{i(M-j)x}\mathbf{e}_j dx. \tag{3.6}$$

Proof. By definition 1.21 on page 12, we will have that $\mathbf{g}_M(t) = \frac{\sin t\sqrt{L}}{\sqrt{L}}\,\mathbf{g}'_M(0)$ and $(\mathbf{g}_M)'_j(0) = \delta_{Mj}$, and so applying theorem 3.10 to $\frac{\sin t\sqrt{L}}{\sqrt{L}}\,\mathbf{g}'_M(0)$ we see

$$\mathbf{g}_M(t) = \frac{1}{\sqrt{2\pi}} \sum_{j\in\mathbb{Z}} \int_0^{2\pi} \frac{\sin\left(tk\sqrt{2(1-\cos x)}\right)}{k\sqrt{2(1-\cos x)}} e^{i(M-j)x}\mathbf{e}_j dx.$$

□

The indexes of the Green's function exhibit a translational symmetry.

Lemma 3.12. *For all* $n \in \mathbb{Z}$*, the Green's functions satisfy* $g_{Mj} = g_{(M+n)(j+n)}$.

Proof. Fix $n \in \mathbb{Z}$. Then

$$g_{(M+n)(j+n)} = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \frac{\sin\left(tk\sqrt{2(1-\cos x)}\right)}{k\sqrt{2(1-\cos x)}} e^{i(M+n-j-n)x} dx = g_{Mj}.$$

□

This translation invariance allows us to restrict our attention to only studying g_0.

Definition 3.12. *Let* G_{0j} *denote the Laplace transform of* g_{0j}.

Lemma 3.13. *The function* $G_{0j}(s)$ *is given by*

$$G_{0j}(s) = \frac{r_+^{|j|}}{-k^2(r_+ - r_-)}, |r_+| < 1, \tag{3.7}$$
$$G_{0j}(s) = \frac{r_-^{|j|}}{-k^2(r_- - r_+)}, |r_+| > 1, \tag{3.8}$$

where $r_\pm = \dfrac{-(s^2+2k^2) \pm \sqrt{s^2(s^2+4k^2)}}{-2k^2}$. *Further,* G_{0j} *is analytic on the right half plane, so the above description uniquely determines* G_{0j}.

Proof. By definition 3.12 and lemma 3.11

$$G_{0j}(s) = \int_0^\infty e^{-st}\frac{1}{2\pi}\int_0^{2\pi} \frac{\sin\left(tk(\sqrt{2-2\cos\xi})\right)}{k\sqrt{2-2\cos\xi}} e^{-ij\xi} d\xi dt.$$

Lets begin by noting the region of absolute convergence: Note that

$$\begin{aligned}
&\int_0^\infty \left| e^{-st}\frac{1}{2\pi}\int_0^{2\pi} \frac{\sin\left(tk(\sqrt{2-2\cos\xi})\right)}{k\sqrt{2-2\cos\xi}} e^{-ij\xi} d\xi \right| dt \\
&\le \int_0^\infty e^{-t\Re s}\frac{1}{2\pi}\int_0^{2\pi} \left| \frac{\sin\left(tk(\sqrt{2-2\cos\xi})\right)}{k\sqrt{2-2\cos\xi}} \right| d\xi dt \\
&\le \int_0^\infty e^{-t\Re s} t dt < \infty,
\end{aligned}$$

whenever $\Re s > 0$. Thus the region of absolute convergence of G_{0j} is $\Re s > 0$, and so G_{0j} is analytic on this region [10]. We can now compute an expression for G_{0j}. Exchanging the order of the integrals we have

$$\begin{aligned}
G_{0j}(s) &= \frac{1}{2\pi}\int_0^{2\pi} \frac{e^{-ij\xi}}{k\sqrt{2-2\cos\xi}}\left[\int_0^\infty e^{-st}\sin\left(tk\sqrt{2-2\cos\xi}\right) dt\right] d\xi \\
&= \frac{1}{2\pi}\int_0^{2\pi} \frac{e^{-ij\xi}}{k\sqrt{2-2\cos\xi}} \frac{k\sqrt{2-2\cos\xi}}{s^2+k^2(2-2\cos\xi)} d\xi \\
&= \frac{1}{2\pi}\int_0^{2\pi} \frac{e^{-ij\xi}}{s^2+2k^2-k^2e^{i\xi}-k^2e^{-i\xi}} d\xi.
\end{aligned}$$

We use the calculus of residues to calculate the above integral. There will be a few cases depending on whether $j \geq 0$ or not, and whether the roots of the polynomial in the denominator of the integrand lay in the unit disk or not. Let $r_\pm$ satisfy

$$r_\pm = \frac{-(s^2+2k^2) \pm \sqrt{s^4+4s^2k^2}}{-2k^2}.$$

Then we have that $(s^2+2k^2)z - k^2 - k^2z^2 = -k^2(z-r_+)(z-r_-)$. Since

$$\begin{aligned} r_+r_- &= \frac{-(s^2+2k^2)+\sqrt{s^4+4s^2k^2}}{-2k^2}\frac{-(s^2+2k^2)-\sqrt{s^4+4s^2k^2}}{-2k^2} \\ &= \frac{s^4+4s^2k^2+4k^4-s^4-4s^2k^2}{4k^4} = \frac{4k^4}{4k^4} = 1, \end{aligned}$$

we may divide the right half plane into three mutually disjoint regions:

$$\begin{aligned} D_1 &= \{s \in \mathbb{C} : \Re s > 0, |r_+(s)| < 1\}, \\ D_2 &= \{s \in \mathbb{C} : \Re s > 0, |r_+(s)| > 1\}, \\ D_3 &= \{s \in \mathbb{C} : \Re s > 0, |r_+(s)| = 1\}. \end{aligned}$$

For the sequel, let $\mathbb{S}$ and $\mathbb{S}_-$ denote the positively and negatively oriented unit circle in $\mathbb{C}$ respectively.

Case 1: Suppose that $s \in D_1$ and $j > 0$. Then set $z = e^{-i\xi}$ so that $dz = -ie^{i\xi}d\xi$, giving

$$\begin{aligned} &\frac{1}{2\pi}\int_0^{2\pi} \frac{e^{-ij\xi}}{s^2+2k^2-k^2e^{i\xi}-k^2e^{-i\xi}}d\xi = \frac{1}{2\pi}\int\limits_{\mathbb{S}_-} \frac{z^j}{s^2+2k^2-k^2\frac{1}{z}-k^2z}\left(\frac{1}{-iz}\right)dz \\ &= \frac{1}{2\pi i}\int\limits_{\mathbb{S}} \frac{z^j}{(s^2+2k^2)z-k^2-k^2z^2}dz. \end{aligned}$$

Since $j > 0$, the value of this integral depends on the location of the roots of the polynomial $(s^2+2k^2)z - k^2 - k^2z^2$. Because $s \in D_1$ by assumption, we automatically have r_+ is contained inside the unit disk and r_- is outside the unit disk (from the relation

$r_+r_- = 1$). The calculus of residues then tells us that for all $s \in D_1$,

$$G_{0j}(s) = \frac{1}{2\pi i}\int\limits_{\mathbb{S}} \frac{z^j}{(s^2+2k^2)z - k^2 - k^2z^2}dz = \text{Res}\left(\frac{z^j}{-k^2(z-r_+)(z-r_-)}, r_+\right) \tag{3.9}$$

$$= \frac{r_+^j}{-k^2(r_+ - r_-)}. \tag{3.10}$$

So for $j > 0$, and $s \in D_1$

$$G_{0j}(s) = \frac{r_+^j}{-k^2(r_+ - r_-)}. \tag{3.11}$$

Case 2: Suppose now that $j < 0$ and $s \in D_1$. Set $z = e^{i\xi}$ so that $dz = ie^{i\xi}d\xi$. Then

$$G_{0j}(s) = \frac{1}{2\pi}\int_0^{2\pi} \frac{e^{-i\xi j}}{s^2 + 2k^2 - k^2e^{i\xi} - k^2e^{-i\xi}}d\xi = \frac{1}{2\pi}\int\limits_{\mathbb{S}} \frac{z^{-j}}{s^2+2k^2-k^2z-k^2\frac{1}{z}}\left(\frac{1}{iz}\right)dz$$

$$= \frac{1}{2\pi i}\int\limits_{\mathbb{S}} \frac{z^{|j|}}{(s^2+2k^2)z - k^2z^2 - k^2}dz.$$

For $j \leq 0$ this is the same exact integral as case 1. So we then see that for $j \leq 0$ and for $s \in D_1$,

$$G_{0j}(s) = \frac{r_+^{|j|}}{-k^2(r_+ - r_-)}.$$

Case 3: Suppose now that $j > 0$ and $s \in D_2$. Set $z = e^{-i\xi}$ so that $dz = -ie^{i\xi}d\xi$ giving

$$\frac{1}{2\pi}\int_0^{2\pi} \frac{e^{-ij\xi}}{s^2 + 2k^2 - k^2e^{i\xi} - k^2e^{-i\xi}}d\xi = \frac{1}{2\pi}\int\limits_{\mathbb{S}_-} \frac{z^j}{s^2+2k^2-k^2\frac{1}{z}-k^2z}\left(\frac{1}{-iz}\right)dz$$

$$= \frac{1}{2\pi i}\int\limits_{\mathbb{S}} \frac{z^j}{(s^2+2k^2)z - k^2 - k^2z^2}dz.$$

Since $j > 0$, the value of this integral depends on the roots of the polynomial $(s^2 +$

$2k^2)z - k^2 - k^2z^2$. Because $s \in D_2$ by assumption, we automatically have r_- is contained inside the unit disk and r_+ is outside the unit disk (from the relation $r_+r_- = 1$). The calculus of residues then tells us that for all $s \in D_2$,

$$G_{0j}(s) = \frac{1}{2\pi i}\int\limits_{\mathbb{S}} \frac{z^j}{(s^2+2k^2)z - k^2 - k^2z^2}dz = \operatorname{Res}\left(\frac{z^j}{-k^2(z-r_+)(z-r_-)}, r_-\right) \tag{3.12}$$

$$= \frac{r_-^j}{-k^2(r_- - r_+)}. \tag{3.13}$$

So for $j > 0$, and $s \in D_2$

$$G_{0j}(s) = \frac{r_-^j}{-k^2(r_- - r_+)}. \tag{3.14}$$

Case 4: Suppose now that $j < 0$ and $s \in D_2$. Set $z = e^{i\xi}$ so that $dz = ie^{i\xi}d\xi$. Then

$$G_{0j}(s) = \frac{1}{2\pi}\int_0^{2\pi} \frac{e^{-i\xi j}}{s^2+2k^2-k^2e^{i\xi}-k^2e^{-i\xi}}d\xi = \frac{1}{2\pi}\int\limits_{\mathbb{S}} \frac{z^{-j}}{s^2+2k^2-k^2z-k^2\frac{1}{z}}\left(\frac{1}{iz}\right)dz$$

$$= \frac{1}{2\pi i}\int\limits_{\mathbb{S}} \frac{z^{|j|}}{(s^2+2k^2)z - k^2z^2 - k^2}dz.$$

For $j \le 0$ this is the same exact integral as case 3. So we then see that for $j \le 0$ and for $s \in D_1$,

$$G_{0j}(s) = \frac{r_-^{|j|}}{-k^2(r_- - r_+)}.$$

Case 5: We will now show that D_3 is empty. Since $r_+r_- = 1$, and since r_+ is the analytic continuation of r_- beyond the curve $x^2 - y^2 + 2k^2 = 0$ in the complex plane, and visa versa, due to the branch cut from the square root, we may simply check that the analytic continuation of $r_-(s)$ never has norm one in the (strict) right half plane. Let R_- be the analytic continuation of $r_-(s)$ to the right half plane (including the imaginary axis).

Then by the maximum modulus principle, the minimum of R_- must lie on the imaginary axis. The branch points of R_- on the imaginary axis are given by $y^4 + 4k^2y^2 = 0$. So $y = 0, 2k, -2k$ are the branch points. For $|y| \leq 2k$ we are on the positive branch of the square root so that

$$|R_-(iy)|^2 = \left| \frac{-y^2 + 2k^2 + \sqrt{y^4 - 4k^2y^2}}{2k^2} \right|^2 = \frac{y^4 - 4k^2y^2 + 4k^4 - y^4 + 4k^2y^2}{4k^4} = 1.$$

When $|y| \geq 2k$, $R_-(s)$ switches branches after hitting the branch point and so the plus in front of the square root becomes a minus:

$$\begin{aligned}
|R_-(iy)|^2 &= \left| \frac{-y^2 + 2k^2 - \sqrt{y^4 - 4k^2y^2}}{2k^2} \right|^2 \\
&= \frac{y^4 - 4k^2y^2 + 4k^4 + y^4 - 4k^2y^2 - 2(2k^2 - y^2)\sqrt{y^4 - 4y^2k^2}}{4k^4} \\
&= 1 + \frac{2y^4 - 8k^2y^2 - 2(2k^2 - y^2)\sqrt{y^4 - 4y^2k^2}}{4k^4} \\
&= 1 + \frac{y^2(y^2 + \sqrt{y^4 - 4k^2} - 4k^2(y^2 + \frac{1}{2}\sqrt{y^4 - 4k^2y^2}}{2k^4}.
\end{aligned}$$

Since $|y| \geq 2k$, we have $y^2(y^2 + \sqrt{y^4 - 4k^2}) \geq 4k^2(y^2 + \frac{1}{2}\sqrt{y^4 - 4k^2y^2})$ giving that $|R_-(iy)|^2 \geq 1$ on this branch. Thus the minimum value of $R_-(s)$ is one, and by the max mod principle all values in the (strict) right half plane must have norm greater than one. This establishes that D_3 is empty. □

Corollary 3.14. *The functions $r_+(s)$ and $r_-(s)$ never have norm one on the right half plane.*

Proof. See the proof of lemma 3.13 on page 56. □

Chapter 4

Relating the Noise and Memory

In equilibrium statistical mechanics, the random noise and memory kernel are connected by the fluctuation dissipation theorem [35]. This chapter establishes a more complicated relationship between noise as defined in definition 1.23 on page 14 and the Laplace transforms of the displacement memory kernel, $\tilde{\beta}$ defined in definition 1.22 on page 14.

Lemma 4.1. *The product of the roots r_+ and r_- satisfy*

$$r_+ r_- = 1. \tag{4.1}$$

Proof. A simple calculation shows

$$\begin{aligned} r_+ r_- &= \frac{-(s^2+2k^2)+\sqrt{s^4+4s^2k^2}}{-2k^2}\frac{-(s^2+2k^2)-\sqrt{s^4+4s^2k^2}}{-2k^2} \\ &= \frac{s^4+4s^2k^2+4k^4-s^4-4s^2k^2}{4k^4} = \frac{4k^4}{4k^4} = 1. \end{aligned}$$

□

Lemma 4.2. *The Green's functions satisfy*

$$G_{0j} = G_{00} r_{\pm}^{|j|}. \tag{4.2}$$

Proof. Using lemma 3.13 on page 56

$$G_{0j} = \frac{r_{\pm}^{|j|}}{-k^2(r_{\pm} - r_{\mp})} = G_{00} r_{\pm}^{|j|},$$

where the plus or minus root is chosen depending on the value of s. $\square$

Lemma 4.3. *The function $\tilde{\beta}$ satisfies*

$$\tilde{\beta} = \frac{1}{r_{\mp}} = r_{\pm}. \tag{4.3}$$

Proof. By definition 1.22 and lemma 4.2.

$$\tilde{\beta} = \frac{k^2 G_{00}}{1 + k^2 G_{01}} = \frac{k^2 \frac{1}{-k^2(r_{\pm} - r_{\mp})}}{1 + k^2 \frac{r_{\pm}}{-k^2(r_{\pm} - r_{\mp})}} = \frac{-1}{r_{\pm} - r_{\pm} - r_{\mp}} = \frac{1}{r_{\mp}} = r_{\pm}.$$

Again the plus or minus depending on whether $s \in D_1$ or D_2. $\square$

Lemma 4.3 on page 63 combined with definition 1.22 and lemma 3.12 on pages 13 and 56 respectively shows that the left and right baths have the same displacement, and thus velocity, memory kernels β and θ. We can now write the Laplace transform of the noise purely in terms of the Laplace transform of displacement memory kernel.

Proposition 4.4. *The noise term $\tilde{F} = \sum_{j \leq 0} \frac{G_{0j} f_j}{1 + k^2 G_{01}}$ satisfies*

$$\tilde{F} = \frac{1}{k^2} \tilde{\beta} \sum_{j \leq 0} \tilde{\beta}^{|j|} f_j. \tag{4.4}$$

Proof. From definition 1.23 and lemmas 4.2 and 4.3 on pages 14, 62, and 63 respectively,

$$\begin{aligned} \tilde{F} &= \sum_{j \leq 0} \frac{G_{0j} f_j}{1 + k^2 G_{01}} = \sum_{j \leq 0} \frac{G_{00} r_{\pm}^{|j|} f_j}{1 + k^2 G_{01}} \\ &= \frac{G_{00}}{1 + k^2 G_{01}} \sum_{j \leq 0} r_{\pm}^{|j|} f_j = \frac{1}{k^2} \beta \sum_{j \leq 0} \beta^{|j|} f_j. \end{aligned}$$

$\square$

This establishes that there is an inherent formal relationship between the memory term and the noise. In order for the relationship to be more than formal however the convergence of the infinite sum defining $\tilde{F}$ must be addressed. It will turn out that the convergence of the sum is computed in the $L^2(\Omega)$ sense, where Ω is the probability space constructed in Chapter 2.

By definition 1.19 and theorem 2.10 on pages 12 and 33, we know each f_j is a mean zero Gaussian random variable, and so the noise term F is a Gaussian mean zero stochastic process. Since mean zero Gaussian processes are uniquely determined by their covariance functions, to determine F we need only calculate the covariance function.

Theorem 4.5. *The Laplace transformed correlation function $\langle \tilde{F}(s)\tilde{F}(s')\rangle$ satisfies*

$$\langle \tilde{F}(s)\tilde{F}(s')\rangle = \frac{k_BT}{k^4}\frac{\tilde{\beta}(s)\tilde{\beta}(s')}{1-\tilde{\beta}(s)\tilde{\beta}(s')}\left[\left(\frac{s}{1-\tilde{\beta}(s)}\right)\left(\frac{s'}{1-\tilde{\beta}(s')}\right)+1\right], \tag{4.5}$$

where $\langle\cdot\rangle$ denotes expected value in Ω.

Proof. For notational convenience, set $x=\tilde{\beta}(s)$, and $y=\tilde{\beta}(s')$. Using lemma 4.4 and theorem 2.10 from pages 63 and 33,

$$\begin{aligned}
&\langle \tilde{F}(s)\tilde{F}(s')\rangle \\
&= \frac{1}{k^4}\left\langle xy\sum_{j,l\le 0} x^{|j|}f_j y^{|l|}f_l\right\rangle \\
&= \frac{xy}{k^4}\sum_{j,l\le 0} x^{|j|}y^{|l|}\langle (su_j(0)+\dot{u}_j(0))(s'u_l(0)+\dot{u}_l(0))\rangle \\
&= \frac{xy}{k^4}\sum_{j,l\le 0} x^{|j|}y^{|l|}(k_BTss'|\max(j,l)-1|+k_BT\delta_{jl}) \\
&= \frac{k_BTxy}{k^4}\left(\sum_{j,l\le 0} x^{|j|}y^{|l|}\delta_{jl} + ss'\sum_{j,l\le 0} x^{|j|}y^{|l|}|\max(j,l)| + ss'\sum_{j,l\le 0} x^{|j|}y^{|l|}\right).
\end{aligned}$$

We can compute this sum piece by piece: Computing the first and last term we find

$$\sum_{j,l\le 0} x^{|j|}y^{|l|}\delta_{jl} = \sum_{j\ge 0}(xy)^j = \frac{1}{1-xy},$$

$$\sum_{j,l\le 0} x^{|j|}y^{|l|} = \left(\sum_{j\ge 0} x^j\right)\left(\sum_{l\ge 0} y^j\right) = \frac{1}{1-x}\frac{1}{1-y}.$$

For the remaining term,

$$\begin{aligned}
&\sum_{j,l\le 0} x^{|j|}y^{|l|}|\max(j,l)| \\
=&\sum_{j,l\ge 0} x^j y^l \min(j,l) \\
=&\sum_{N=1}^{\infty} y^N \left(\sum_{j=1}^{N-1} jx^j + N\sum_{j=N}^{\infty} x^j\right) \\
=&\sum_{N=1}^{\infty} y^N \left[\frac{(N-1)x^{N+1} - Nx^N + x}{(1-x)^2} + N\frac{x^N}{1-x}\right] \\
=&\frac{x}{(1-x)^2}\sum_{N=1}^{\infty} y^N x^N (N-1) - \frac{1}{(1-x)^2}\sum_{N=1}^{\infty} Ny^N x^N + \\
&\quad \frac{x}{(1-x)^2}\sum_{N=1}^{\infty} y^N + \frac{1}{1-x}\sum_{N=1}^{\infty} Nx^N y^N \\
=&\frac{x}{(1-x)^2}\frac{x^2y^2}{(1-xy)^2} - \frac{1}{(1-x)^2}\frac{xy}{(1-xy)^2} + \frac{x}{(1-x)^2}\frac{y}{1-y} + \frac{1}{1-x}\frac{xy}{(1-xy)^2} \\
=&\frac{x^3y^2}{(1-x)^2(1-xy)^2} - \frac{xy}{(1-x)^2(1-xy)^2} + \frac{xy}{(1-x)^2(1-y)} + \frac{xy}{(1-x)(1-xy)^2} \\
=&\frac{xy}{1-x}\left[\frac{x^2y}{(1-x)(1-xy)^2} - \frac{1}{(1-x)(1-xy)^2} + \frac{1}{(1-x)(1-y)} + \frac{1}{(1-xy)^2}\right] \\
=&\frac{xy}{1-x}\left[\frac{x^2y(1-y)}{(1-x)(1-xy)^2(1-y)} - \frac{1-y}{(1-x)(1-xy)^2(1-y)}\right. \\
&\qquad\left. + \frac{(1-xy)^2}{(1-x)(1-xy)^2(1-y)} + \frac{(1-x)(1-y)}{(1-x)(1-xy)^2(1-y)}\right] \\
=&\frac{xy}{(1-x)^2(1-xy)^2(1-y)}\left[x^2y - x^2y^2 - 1 + y + 1 - 2xy + x^2y^2 + 1 - x - y + xy\right] \\
=&\frac{xy}{(1-x)^2(1-xy)^2(1-y)}\left[x^2y + 1 - xy - x\right] \\
=&\frac{xy}{(1-x)^2(1-xy)^2(1-y)}\left[(1-x)(1-xy)\right]
\end{aligned}$$

$$=\frac{xy}{(1-x)(1-y)(1-xy)}.$$

We can now begin to put this all together. Note that

$$\begin{aligned}
&ss'\sum_{j,l\leq 0} x^{|j|}y^{|l|}|\max(j,l)| + ss'\sum_{j,l\leq 0} x^{|j|}y^{|l|}\\
&= ss'\left(\frac{1}{1-x}\frac{1}{1-y} + \frac{xy}{(1-x)(1-y)(1-xy)}\right)\\
&= ss'\left(\frac{xy+1-xy}{(1-x)(1-y)(1-xy)}\right)\\
&= \frac{ss'}{(1-x)(1-y)(1-xy)}.
\end{aligned}$$

Combining with the first term then gives,

$$\begin{aligned}
\langle \tilde{F}(s)\tilde{F}(s')\rangle &= \frac{k_BTxy}{k^4}\left(\frac{1}{1-xy} + \frac{ss'}{(1-x)(1-y)(1-xy)}\right)\\
&= \frac{k_BTxy}{k^4(1-xy)}\left(\frac{s}{1-x}\frac{s'}{1-y} + 1\right).
\end{aligned}$$

□

In particular this shows that for each fixed $s \in \mathbb{C}, \Re(s) > 0$, $\tilde{F}(s) \in L^2(\Omega)$, where $\Re(s)$ denotes the real part of s. Theorem 4.5 will ultimately show that the noise is not stationary. To do this we compute what the noise should be if it were stationary in time domain. Then transform that function back to Laplace space and compare the result against theorem 4.5 on page 64. If the two results are different, the noise cannot be stationary. First though, a lemma of some minor results that will help simplify the tediousness of the calculations.

Lemma 4.6. *The memory kernel β, and its Laplace transform $\tilde{\beta}$ satisfy:*

- $$\lim_{s\to\infty} \tilde{\beta}(s) = 0,$$

- $$\beta(0) = \lim_{s\to\infty} s\tilde{\beta}(s) = 0,$$

- $$\lim_{s\to\infty} s^2\tilde{\beta}(s) = k^2.$$

Proof. These are all just straightforward calculations:

$$\lim_{s\to\infty} \tilde{\beta}(s) = \lim_{s\to\infty} \frac{2k^2}{s^2 + 2k^2 + \sqrt{s^4 + 4s^2k^2}} = 0.$$

The initial value theorem for Laplace transforms [10] gives that $\lim_{s\to\infty} s\tilde{\beta}(s) = \beta(0)$. Using this and calculating the limit we have

$$\begin{aligned}\beta(0) &= \lim_{s\to\infty} s\tilde{\beta}(s) \\ &= \lim_{s\to\infty} \frac{2k^2 s}{s^2 + 2k^2 + \sqrt{s^4 + 4s^2k^2}} = \lim_{s\to\infty} \frac{2k^2}{s + \frac{2k^2}{s} + \sqrt{s^2 + 4k^2}} = 0.\end{aligned}$$

Lastly we find,

$$\begin{aligned}\lim_{s\to\infty} s^2\tilde{\beta}(s) &= \lim_{s\to\infty} \frac{2s^2k^2}{s^2 + 2k^2 + \sqrt{s^4 + 4s^2k^2}} \\ = \lim_{s\to\infty} &\frac{2k^2}{1 + \frac{2k^2}{s^2} + \sqrt{1 + \frac{4k^2}{s^2}}} = \frac{2k^2}{2} = k^2.\end{aligned}$$

□

We now compute the correlation function $\langle F(0)F(t)\rangle$.

Theorem 4.7. *The noise satisfies the relationship:*

$$\langle F(0)F(t)\rangle = k_B T \frac{J_1(2kt)}{kt}, \tag{4.6}$$

where J_1 is the first Bessel function of the first kind.

Proof. First we show

$$\langle F(0)\tilde{F}(s)\rangle = \frac{k_B T s\tilde{\beta}(s)}{k^2(1-\tilde{\beta}(s))}.$$

Again using the initial value theorem of Laplace transforms and the lemma 4.6

$$\begin{aligned}
&\langle F(0)\tilde{F}(\sigma) = \lim_{s\to\infty}\langle s\langle \tilde{F}(s)\tilde{F}(\sigma)\rangle \\
=&\frac{k_B T}{k^4}\tilde{\beta}(\sigma)\left[\frac{s\tilde{\beta}(s)}{1-\tilde{\beta}(s)\tilde{\beta}(\sigma)}\left(\frac{s}{1-\tilde{\beta}(s)}\frac{\sigma}{1-\tilde{\beta}(\sigma)}+1\right)\right] \\
=&\frac{k_B T\tilde{\beta(\sigma)}}{k^4}\lim_{s\to\infty}\left[s\tilde{\beta}(s)\left(s\frac{\sigma}{1-\tilde{\beta}(\sigma)}+1\right)\right] \\
=&\frac{k_B T\tilde{\beta}(\sigma)}{k^4}\lim_{s\to\infty}\left(s^2\tilde{\beta}(s)\frac{\sigma}{1-\tilde{\beta}(\sigma)}+s\tilde{\beta}(s)\right) \\
=&\frac{k_B T}{k^4}\frac{\sigma\tilde{\beta}(\sigma)}{1-\tilde{\beta}(\sigma)}\lim_{s\to\infty}s^2\tilde{\beta}(s) \\
=&\frac{k_B T}{k^4}\frac{\sigma\tilde{\beta}(\sigma)}{1-\tilde{\beta}(\sigma)}k^2 = \frac{k_B T}{k^2}\frac{\sigma\tilde{\beta}(\sigma)}{1-\tilde{\beta}(\sigma)}.
\end{aligned}$$

However,

$$\begin{aligned}
&\frac{1}{k^2}\frac{s\tilde{\beta}(s)}{1-\tilde{\beta}(s)} \\
=&\frac{1}{k^2}\left[\frac{\frac{2k^2 s}{s^2+2k^2+\sqrt{s^4+4s^2k^2}}}{1-\frac{2k^2}{s^2+2k^2+\sqrt{s^4+4s^2k^2}}}\right] \\
=&\frac{\frac{2s}{s^2+2k^2+\sqrt{s^4+4s^2k^2}}}{\frac{s^2+\sqrt{s^4+4s^2k^2}}{s^2+2k^2+\sqrt{s^4+4s^2k^2}}} \\
=&\frac{2s}{s^2+\sqrt{s^4+4s^2k^2}} \\
=&\frac{2}{s+\sqrt{s^2+4k^2}} \\
=&\frac{2\left(s-\sqrt{s^2+4k^2}\right)}{s^2-s^2-4k^2} = \frac{\sqrt{s^2+4k^2}-s}{2k^2}.
\end{aligned}$$

Using the lookup table [26], $\dfrac{\sqrt{s^2+4k^2}-s}{2k^2}$ is the Laplace transform of $\frac{J_1(2kt)}{kt}$. Hence

$\langle F(0)F(t)\rangle = k_B T \dfrac{J_1(2kt)}{kt}$, completing the proof. $\square$

Recall from definition 1.24 on page 15, $\theta(t) := \int_t^\infty \beta(\tau)d\tau$.

Lemma 4.8. *The velocity memory kernel, $\theta(t)$ satisfies*

$$\theta(t) = \frac{J_1(2kt)}{kt}. \tag{4.7}$$

Proof. In Laplace space, $\tilde{\theta}(s) = \frac{1}{s}\theta(0) - \frac{1}{s}\tilde{\beta}(s)$. By the initial value theorem of Laplace transforms,

$$\theta(0) = \int_0^\infty \beta(\tau)d\tau = \lim_{s\to 0}\tilde{\beta}(s).$$

Computing the limit we find

$$\lim_{s\to 0}\tilde{\beta}(s) = \lim_{s\to 0}\frac{2k^2}{s^2+2k^2+\sqrt{s^4+4k^2s^2}} = \frac{2k^2}{2k^2} = 1,$$

establishing $\tilde{\theta}(s) = \dfrac{1}{s}\left(1-\tilde{\beta}(s)\right)$. Simplifying

$$\begin{aligned}
\tilde{\theta}(s) &= \frac{1}{s}\left(1-\tilde{\beta}(s)\right) = \frac{1}{s}\left(1-\frac{2k^2}{s^2+2k^2+\sqrt{s^4+4k^2s^2}}\right)\\
&= \frac{1}{s}\left(1-\frac{s^2+2k^2-\sqrt{s^4+4s^2k^2}}{2k^2}\right)\\
&= \frac{1}{s}\left(1-1+\frac{s^2-\sqrt{s^4+4k^2s^2}}{2k^2}\right)\\
&= \frac{\sqrt{s^2+4k^2}-s}{2k^2}.
\end{aligned}$$

This is the same inversion as in the proof of theorem 4.7 on page 67. $\square$

Corollary 4.9. *The noise and memory terms satisfy*

$$\langle F(0)F(t)\rangle = k_B T\theta(t). \tag{4.8}$$

Proof. Combine theorems 4.7, and lemma 4.8 from pages 67 and 69 respectively. □

Lemma 4.10. *The function $\theta(t_1 - t_2)$ has double Laplace transform*

$$\frac{1}{s_1 + s_2}\left[\frac{-s_1 + \sqrt{s_1^2 + 4k^2}}{2k^2} + \frac{-s_2 + \sqrt{s_2^2 + 4k^2}}{2k^2}\right]. \tag{4.9}$$

Proof. The Taylor series expansion of $J_1(t)$ gives

$$\theta(t_1 - t_2) = \frac{1}{k(t_1 - t_2)} \sum_{m=0}^{\infty} \frac{(-1)^m}{m!(m+1)!} \left(\frac{2k(t_1 - t_2)}{2}\right)^{2m+1} = \sum_{m=0}^{\infty} \frac{(-1)^m k^{2m}}{m!(m+1)!} (t_1 - t_2)^{2m}.$$

Taking the double Laplace transform we find

$$\begin{aligned}
&\int_{t_1=0}^{t_1=\infty} \int_{t_2=0}^{t_2=\infty} e^{-s_1 t_1 - s_2 t_2} \sum_{m=0}^{\infty} \frac{(-1)^m k^{2m}}{m!(m+1)!} (t_1 - t_2)^{2m} \, dt_1 dt_2 \\
&= \sum_{m=0}^{\infty} \frac{(-1)^m k^{2m}}{m!(m+1)!} \int_{t_1=0}^{t_1=\infty} \int_{t_2=0}^{t_2=\infty} e^{-s_1 t_1 - s_2 t_2} (t_1 - t_2)^{2m} \, dt_1 dt_2 \\
&= \sum_{m=0}^{\infty} \frac{(-1)^m k^{2m}}{m!(m+1)!} \frac{\left[(2m)! s_1^{-1-2m} \left[1 + \frac{s_1 \left(\frac{-s_2}{s_1}\right)^{-2m}}{s_2}\right]\right]}{s_1 + s_2} \\
&= \sum_{m=0}^{\infty} \frac{(-1)^m k^{2m} (2m)!}{m!(m+1)!} \left[\frac{s_1^{-2m-1} + s_2^{-2m-1}}{s_1 + s_2}\right] \\
&= \frac{1}{s_1 + s_2} \sum_{m=0}^{\infty} \frac{(-1)^m k^{2m} (2m)!}{m!(m+1)!} \left[s_1^{-2m-1} + s_2^{-2m-1}\right] \\
&= \frac{1}{s_1 + s_2} \left[\sum_{m=0}^{\infty} \frac{(-1)^m k^{2m} (2m)!}{m!(m+1)!} s_1^{-2m-1} + \sum_{m=0}^{\infty} \frac{(-1)^m k^{2m} (2m)!}{m!(m+1)!} s_2^{-2m-1}\right].
\end{aligned}$$

These two series have known closed forms:

$$= \frac{1}{s_1 + s_2} \left[\sum_{m=0}^{\infty} \frac{(-1)^m k^{2m} (2m)!}{m!(m+1)!} s_1^{-2m-1} + \sum_{m=0}^{\infty} \frac{(-1)^m k^{2m} (2m)!}{m!(m+1)!} s_2^{-2m-1}\right]$$

$$
\begin{aligned}
&= \frac{1}{s_1+s_2}\left[\frac{s_1\left(-1+\sqrt{\frac{4k^2}{s_1^2}+1}\right)}{2k^2}+\frac{s_2\left(-1+\sqrt{\frac{4k^2}{s_2^2}+1}\right)}{2k^2}\right] \\
&= \frac{1}{s_1+s_2}\left[\frac{-s_1+\sqrt{s_1^2+4k^2}}{2k^2}+\frac{-s_2+\sqrt{s_2^2+4k^2}}{2k^2}\right].
\end{aligned}
$$

□

To make the following argument easier, it is useful to introduce some additional notation and prove some minor computational lemmas:

Definition 4.1. *The function $\gamma(s)$ is defined by*

$$
\gamma(s) := \tilde{\beta}(s) - 1 = \frac{s^2 - \sqrt{s^4+4k^2s^2}}{2k^2}. \tag{4.10}
$$

Definition 4.2. *The algebraic conjugate of $\gamma(s)$, denoted $\overline{\gamma}(s)$ is defined by*

$$
\overline{\gamma}(s) = \frac{s^2 + \sqrt{s^4+4k^2s^2}}{2k^2}. \tag{4.11}
$$

Lemma 4.11. *The function γ and its algebraic conjugate $\overline{\gamma}$ satisfy:*

1. $\dfrac{1}{\gamma(s)} = \dfrac{-k^2}{s^2}.\overline{\gamma}(s)$
2. $\gamma(s)\overline{\gamma}(s) = -\frac{s^2}{k^2}$.
3. $\frac{k^4}{s_1 s_2}\overline{\gamma}(s_1)\overline{\gamma}(s_2)$
   $= \frac{1}{4}\left[s_1s_2 + s_1\sqrt{s_2^2+4k^2} + s_2\sqrt{s_1^2+4k^2} + \sqrt{s_1^2+4k^2}\sqrt{s_2^2+4k^2}\right].$

Proof. Direct calculations from definitions 4.1 and 4.2 show

$$
\begin{aligned}
\frac{1}{\gamma(s)} &= \frac{2k^2}{s^2-\sqrt{s^4+4k^2s^2}} = \frac{2k^2(s^2+\sqrt{s^4+4k^2s^2})}{s^4-s^4-4k^2s^2} \\
&= \frac{s^2+\sqrt{s^4+4k^2s^2}}{-2s^2} = \frac{-k^2}{s^2}\overline{\gamma}(s).
\end{aligned}
$$

Similarly,

$$\gamma(s)\overline{\gamma}(s) = \frac{s^2 - \sqrt{s^4 + 4k^2 s^2}}{2k^2} \frac{s^2 + \sqrt{s^4 + 4k^2 s^2}}{2k^2} = \frac{s^4 - s^4 - 4k^2 s^2}{4k^4} = -\frac{s^2}{k^2}.$$

Finally,

$$\begin{aligned}
&\frac{k^4}{s_1 s_2}\overline{\gamma}(s_1)\overline{\gamma}(s_2) = \frac{k^4}{s_1 s_2}\left[\frac{s_1^2 + \sqrt{s_1^4 + 4k^2 s_1^2}}{2k^2}\right]\left[\frac{s_2^2 + \sqrt{s_2^4 + 4k^2 s_2^2}}{2k^2}\right] \\
&= \frac{1}{4}\left(s_1 + \sqrt{s_1^2 + 4k^2}\right)\left(s_2 + \sqrt{s_2^2 + 4k^2}\right) \\
&= \frac{1}{4}\left[s_1 s_2 + s_1\sqrt{s_2^2 + 4k^2} + s_2\sqrt{s_1^2 + 4k^2} + \sqrt{s_1^2 + 4k^2}\sqrt{s_2^2 + 4k^2}\right].
\end{aligned}$$

□

Theorem 4.12. *The double Laplace transform of the correlation function satisfies*

$$\begin{aligned}
&\langle \tilde{F}(s_1)\tilde{F}(s_2)\rangle \\
=&\frac{-1}{2k^4(s_2^2 - s_1^2)}\left[s_2(s_2 - \sqrt{s_2^2 + 4k^4}) - s_1(s_1 - \sqrt{s_1^2 + 4k^2})\right. \\
&\left. -k^2 s_2\sqrt{s_1^2 + 4k^2} + k^2 s_1\sqrt{s_2^2 + 4k^2}\right].
\end{aligned}$$

Proof. Using the theorem 4.5, definitions 4.1 and 4.2, and lemma 4.11 from pages 64 and 71,

$$\begin{aligned}
\langle \tilde{F}(s_1)\tilde{F}(s_2)\rangle &= \frac{1}{k^4}\frac{(\gamma(s_1)+1)(\gamma(s_2)+1)}{1-(\gamma(s_1)+1)(\gamma(s_2)+1)}\left[\frac{s_1}{1-(\gamma(s_1)+1)}\frac{s_2}{1-(\gamma(s_2)+1)} + 1\right] \\
&= \frac{1}{k^4}\left[\frac{\gamma(s_1)\gamma(s_2)+\gamma(s_1)+\gamma(s_2)+1}{-\gamma(s_1)\gamma(s_2)-\gamma(s_1)-\gamma(s_2)}\right]\left[\frac{s_1}{-\gamma(s_1)}\frac{s_2}{-\gamma(s_2)} + 1\right] \\
&= \frac{-1}{k^4}\left[\frac{\gamma(s_1)\gamma(s_2)+\gamma(s_1)+\gamma(s_2)+1}{\gamma(s_1)\gamma(s_2)+\gamma(s_1)+\gamma(s_2)}\right]\left[\left(-s_1\frac{-k^2}{s_1^2}\overline{\gamma}(s_1)\right)\left(-s_2\frac{-k^2}{s_2^2}\overline{\gamma}(s_2)\right) + 1\right] \\
&= \frac{-1}{k^4}\left[\frac{\gamma(s_1)\gamma(s_2)+\gamma(s_1)+\gamma(s_2)+1}{\gamma(s_1)\gamma(s_2)+\gamma(s_1)+\gamma(s_2)}\right]\left[\frac{k^2}{s_1}\overline{\gamma}(s_1)\frac{k^2}{s_2}\overline{\gamma}(s_2) + 1\right]
\end{aligned}$$

$$
\begin{aligned}
&= \frac{-1}{k^4}\left[\frac{k^4}{s_1 s_2}\gamma(s_1)\gamma(s_2)\overline{\gamma}(s_1)\overline{\gamma}(s_2) + \frac{k^4}{s_1 s_2}\gamma(s_1)\overline{\gamma}(s_1)\overline{\gamma}(s_2)\right.\\
&\quad + \frac{k^4}{s_1 s_2}\gamma(s_2)\overline{\gamma}(s_1)\overline{\gamma}(s_2) + \frac{k^4}{s_1 s_2}\overline{\gamma}(s_1)\overline{\gamma}(s_2)\\
&\quad \left.+\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2) + 1\right] / \left[\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)\right]\\
&= \frac{-1}{k^4}\left[1 + \left[\frac{k^4}{s_1 s_2}\left(\frac{-s_1^2}{k^2}\right)\left(\frac{-s_2^2}{k^2}\right) + \frac{k^4}{s_1 s_2}\left(\frac{-s_1^2}{k^2}\right)\overline{\gamma}(s_2)\right.\right.\\
&\quad \left.\left.+\frac{k^4}{s_1 s_2}\left(\frac{-s_2^2}{k^2}\right)\overline{\gamma}(s_1) + \frac{k^4}{s_1 s_2}\overline{\gamma}(s_1)\overline{\gamma}(s_2) + 1\right] / \left[\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)\right]\right]\\
&= \frac{-1}{k^4}\left[1 + \frac{s_1 s_2 - \frac{k^2 s_1}{s_2}\left(\frac{s_2^2+\sqrt{s_2^4+4k^2 s_2^2}}{2k^2}\right) - \frac{k^2 s_2}{s_1}\left(\frac{s_1^2+\sqrt{s_1^4+4k^2 s_1^2}}{2k^2}\right) + \frac{k^4}{s_1 s_2}\overline{\gamma}(s_1)\overline{\gamma}(s_2) + 1}{\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)}\right]\\
&= \frac{-1}{k^4}\left[1 + \frac{s_1 s_2 - \frac{s_1 s_2 + s_1\sqrt{s_2^2+4k^2}}{2} - \frac{s_2 s_1 + s_2\sqrt{s_1^2+4k^2}}{2} + \frac{k^4}{s_1 s_2}\overline{\gamma}(s_1)\overline{\gamma}(s_2) + 1}{\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)}\right]\\
&= \frac{-1}{k^4}\left[1 + \left[s_1 s_2 - \frac{s_1 s_2}{2} - \frac{s_1\sqrt{s_2^2+4k^2}}{2} - \frac{s_1 s_2}{2} - \frac{s_2\sqrt{s_1^2+4k^2}}{2}\right.\right.\\
&\quad + \frac{s_1 s_2}{4} + \frac{s_1\sqrt{s_2^2+4k^2}}{4} + \frac{s_2\sqrt{s_1^2+4k^2}}{4}\\
&\quad \left.\left.+\frac{\sqrt{s_1^2+4k^2}\sqrt{s_2^2+4k^2}}{4} + 1\right] / \left[\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)\right]\right]\\
&= \frac{-1}{k^4}\left[1 + \frac{\frac{s_1 s_2}{4} - \frac{s_1\sqrt{s_2+4k^2}}{4} - \frac{s_2\sqrt{s_1^2+4k^2}}{4} + \frac{\sqrt{s_1^2+4k^2}\sqrt{s_2^2+4k^2}}{4} + 1}{\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)}\right]\\
&= \frac{-1}{k^4}\left[1 + \frac{\left(\frac{s_1-\sqrt{s_1^2+4k^2}}{2}\right)\left(\frac{s_2-\sqrt{s_2^2+4k^2}}{2}\right) + 1}{\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)}\right]
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{-1}{k^4}\left[1 + \frac{\frac{k^2\gamma(s_1)}{s_1}\frac{k^2\gamma(s_2)}{s_2} + 1}{\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)}\right]\\
&= \frac{-1}{k^4}\left[1 + \frac{k^4\frac{\gamma(s_1)\gamma(s_2)}{s_1 s_2} + 1}{\gamma(s_1)\gamma(s_2) + \gamma(s_1) + \gamma(s_2)}\right]\\
&= \frac{-1}{k^4}\left[1 + \frac{1 + \frac{s_1 s_2}{k^4\gamma(s_1)\gamma(s_2)}}{\left[1 + \frac{1}{\gamma(s_1)} + \frac{1}{\gamma(s_2)}\right]\frac{s_1 s_2}{k^4}}\right]
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{-1}{k^4}\left[1+\frac{\frac{s_1s_2}{k^4}\frac{k^4}{s_1s_2}\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{\left[1-\frac{k^2}{s_1^2}\overline{\gamma}(s_1)-\frac{k^2}{s_2^2}\overline{\gamma}(s_2)\right]\frac{s_1s_2}{k^4}}\right]\\
&= \frac{-1}{k^4}\left[1+\frac{1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}}{\frac{s_1s_2}{k^4}-\frac{k^2s_2}{k^4s_1}\overline{\gamma}(s_1)-\frac{k^2s_1}{k^4s_2}\overline{\gamma}(s_2)}\right]\\
&= \frac{-1}{k^4}\left[1+\frac{1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}}{\frac{s_1s_2}{k^4}-\frac{k^2s_2}{k^4s_1}\left(\frac{s_1^2+\sqrt{s_1^4+4k^2s_1^2}}{2k^2}\right)-\frac{k^2s_1}{k^4s_2}\left(\frac{s_2^2+\sqrt{s_2^4+4k^2s_2^2}}{2k^2}\right)}\right]\\
&= \frac{-1}{k^4}\left[1+\frac{1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}}{\frac{s_1s_2}{k^4}-\frac{s_2s_1}{2k^4}-\frac{s_2\sqrt{s_1^2+4k^2}}{2k^4}-\frac{s_1s_2}{2k^4}-\frac{s_1\sqrt{s_2^2+4k^2}}{2k^4}}\right]\\
&= \frac{-1}{k^4}\left[1+\frac{1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}}{\left(\frac{-s_2\sqrt{s_1^2+4k^2}-s_1\sqrt{s_2^2+4k^2}}{2k^4}\right)}\right]\\
&= \frac{-1}{k^4}\left[1-2k^4\left[\frac{1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}}{s_2\sqrt{s_1^2+4k^2}+s_1\sqrt{s_2^2+4k^2}}\right]\right]\\
&= \frac{-1}{k^2}\left[1-2k^4\left[\frac{\left(1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}\right)\left(s_2\sqrt{s_1^2+4k^2}-s_1\sqrt{s_2^2+4k^2}\right)}{\left(s_2\sqrt{s_1^2+4k^2}+s_1\sqrt{s_2^2+4k^2}\right)\left(s_2\sqrt{s_1^2+4k^2}-s_1\sqrt{s_2^2+4k^2}\right)}\right]\right]\\
&= \frac{-1}{k^2}\left[1-2k^4\left[\frac{\left(1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}\right)\left(s_2\sqrt{s_1^2+4k^2}-s_1\sqrt{s_2^2+4k^2}\right)}{s_2^2(s_1^2+4k^2)-s_1^2(s_2^2+4k^2)}\right]\right]\\
&= \frac{-1}{k^2}\left[1-2k^4\left[\frac{\left(1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}\right)\left(s_2\sqrt{s_1^2+4k^2}-s_1\sqrt{s_2^2+4k^2}\right)}{4k^2(s_2^2-s_1^2)}\right]\right]\\
&= \frac{-1}{k^2}\left[1-k^4\left[\frac{\left(1+\frac{\overline{\gamma}(s_1)\overline{\gamma}(s_2)}{s_1s_2}\right)\left(s_2\sqrt{s_1^2+4k^2}-s_1\sqrt{s_2^2+4k^2}\right)}{2k^2(s_2^2-s_1^2)}\right]\right]
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{-1}{k^2 2k^2(s_2^2-s_1^2)}\Bigg[2k^2s_2^2-2k^2s_1^2-k^4\Bigg[\left(s_2\sqrt{s_1^2+4k^2}-s_1\sqrt{s_2^2+4k^2}\right)\\
&\qquad\times\left(1+\frac{s_1s_2}{4k^4}+\frac{s_1}{4k^4}\sqrt{s_2^2+4k^2}+\frac{s_2}{4k^4}\sqrt{s_1^2+4k^2}+\frac{1}{4k^4}\sqrt{s_1^2+4k^2}\sqrt{s_2^2+4k^2}\right)\Bigg]\Bigg]\\
&= \frac{-1}{2k^6(s_2^2-s_1^2)}\Bigg[2k^2s_2^2-2k^2s_1^2-\Bigg[k^4s_2\sqrt{s_1^2+4k^2}+s_1s_2^2\sqrt{s_1^2+4k^2}\\
&\qquad+s_1s_2\sqrt{s_1^2+4k^2}\sqrt{s_2^2+4k^2}+s_2^2(s_1^2+4k^2)+s_2\sqrt{s_1^2+4k^2}(s_1^2+4k^2)
\end{aligned}
$$

$$-k^4 s_1\sqrt{s_2^2+4k^2} - s_1^2 s_2\sqrt{s_2^2+4k^2} - s_1^2(s_2^2+4k^2)$$

$$-s_1 s_2\sqrt{s_1^2+4k^2}\sqrt{s_2^2+4k^2} - s_1\sqrt{s_1^2+4k^2}(s_2^2+4k^2)\Big]\Big]$$

$$= \frac{-1}{2k^6(s_2^2-s_1^2)}\Big[2k^2s_2^2 - 2k^2s_1^2 - k^4 s_2\sqrt{s_1^2+4k^2} - s_1 s_2^2\sqrt{s_1^2+4k^2}$$

$$-s_1 s_2\sqrt{s_1^2+4k^2}\sqrt{s_2^2+4k^2} - s_2^2 s_1^2 - s_2^2 4k^2 - s_2\sqrt{s_1^2+4k^2}s_1^2 - 4k^2 s_2\sqrt{s_1^2+4k^2}$$

$$+k^4 s_1\sqrt{s_2^2+4k^2} + s_1^2 s_2\sqrt{s_2^2+4k^2} + s_1^2 s_2^2 + 4k^2 s_2^2$$

$$+s_1 s_2\sqrt{s_1^2+4k^2}\sqrt{s_2^2+4k^2} + s_1\sqrt{s_1^2+4k^2}s_2^2 + 4k^2 s_1\sqrt{s_1^2+4k^2}\Big]$$

$$= \frac{-1}{2k^6(s_2^2-s_1^2)}\Big[k^2s_2^2 - k^2s_1^2 - k^4 s_2\sqrt{s_1^2+4k^2} + k^4 s_1\sqrt{s_2^2+4k^2}$$

$$-k^2 s_2\sqrt{s_2^2+4k^4} + k^2 s_1\sqrt{s_1^2+4k^2}\Big]$$

$$= \frac{-1}{2k^4(s_2^2-s_1^2)}\Big[s_2^2 - s_1^2 - k^2 s_2\sqrt{s_1^2+4k^2} + k^2 s_1\sqrt{s_2^2+4k^2}$$

$$-s_2\sqrt{s_2^2+4k^4} + s_1\sqrt{s_1^2+4k^2}\Big]$$

$$= \frac{-1}{2k^4(s_2^2-s_1^2)}\Big[s_2\left(s_2 - \sqrt{s_2^2+4k^4}\right)$$

$$-s_1\left(s_1 - \sqrt{s_1^2+4k^2}\right) - k^2 s_2\sqrt{s_1^2+4k^2} + k^2 s_1\sqrt{s_2^2+4k^2}\Big].$$

□

We can finally compare the difference in Laplace space between the double Laplace transform of the correlation function and the double Laplace transform of the memory kernel.

Corollary 4.13. *Let Lap denote the 2d Laplace transform. Then*

$$\tilde{D}(s_1,s_2) := \langle \tilde{F}(s_1)\tilde{F}(s_2)\rangle - Lap\,(\theta(t_1-t_2))\,(s_1,s_2) \tag{4.12}$$

$$= \frac{k^2-1}{k^2(s_2^2-s_1^2)}\left[\frac{s_2(s_2-\sqrt{s_2^2+4k^2})}{2k^2} - \frac{s_1(s_1-\sqrt{s_1^2+4k^2})}{2k^2}\right]. \tag{4.13}$$

In particular the noise term F cannot be stationary.

Proof. Using theorem 4.12 and lemma 4.10 from pages 72 and 70, computing the difference we find

$$
\begin{aligned}
&\frac{-1}{2k^4(s_2^2-s_1^2)}\left[s_2\left(s_2-\sqrt{s_2^2+4k^4}\right)-s_1\left(s_1-\sqrt{s_1^2+4k^2}\right)\right.\\
&\quad\left.-k^2s_2\sqrt{s_1^2+4k^2}+k^2s_1\sqrt{s_2^2+4k^2}\right]\\
&-\frac{1}{2k^2(s_1+s_2)}\left[-s_1+\sqrt{s_1^2+4k^2}-s_2+\sqrt{4k^2+s_2^2}\right]\\
&=\frac{-1}{2k^4(s_2^2-s_1^2)}\left[s_2\left(s_2-\sqrt{s_2^2+4k^4}\right)-s_1\left(s_1-\sqrt{s_1^2+4k^2}\right)\right.\\
&\quad-k^2s_2\sqrt{s_1^2+4k^2}+k^2s_1\sqrt{s_2^2+4k^2}\\
&\quad\quad\left.+k^2(s_2-s_1)\left[-s_1+\sqrt{s_1^2+4k^2}-s_2+\sqrt{s_2^2+4k^2}\right]\right]\\
&=\frac{-1}{2k^4(s_2^2-s_1^2)}\left[s_2\left(s_2-\sqrt{s_2^2+4k^4}\right)-s_1\left(s_1-\sqrt{s_1^2+4k^2}\right)\right.\\
&\quad-k^2s_2\sqrt{s_1^2+4k^2}+k^2s_1\sqrt{s_2^2+4k^2}\\
&\quad\quad-k^2s_2s_1+k^2s_2\sqrt{s_1^2+4k^2}-k^2s_2^2+k^2s_2\sqrt{s_2^2+4k^2}\\
&\quad\quad\left.+k^2s_1^2-k^2s_1\sqrt{s_1^2+4k^2}+k^2s_1s_2-s_1\sqrt{s_2^2+4k^2}\right]\\
&=\frac{-1}{2k^4(s_2^2-s_1^2)}\left[s_2\left(s_2-\sqrt{s_2^2+4k^4}\right)-s_1\left(s_1-\sqrt{s_1^2+4k^2}\right)\right.\\
&\quad\quad\left.-k^2s_2^2+k^2s_2\sqrt{s_2^2+4k^2}+k^2s_1^2-k^2s_1\sqrt{s_1^2+4k^2}\right]\\
&=\frac{-1}{2k^4(s_2^2-s_1^2)}\left[s_2\left(s_2-\sqrt{s_2^2+4k^4}\right)-s_1\left(s_1-\sqrt{s_1^2+4k^2}\right)\right.\\
&\quad\quad\left.-k^2s_2\left(s_2-\sqrt{s_2^2+4k^2}\right)+k^2s_1\left(s_1-\sqrt{s_1^2+4k^2}\right)\right]\\
&=\frac{-(1-k^2)}{2k^4(s_2^2-s_1^2)}\left[s_2\left(s_2-\sqrt{s_2^2+4k^2}\right)-s_1\left(s_1-\sqrt{s_1^2+4k^2}\right)\right]\\
&=\frac{k^2-1}{k^2(s_2^2-s_1^2)}\left[\frac{s_2(s_2-\sqrt{s_2^2+4k^2})}{2k^2}-\frac{s_1(s_1-\sqrt{s_1^2+4k^2})}{2k^2}\right].
\end{aligned}
$$

Since $\tilde{D}$ is non-zero, the noise cannot possibly be stationary. □

Chapter 5

Existence Theory

Before we begin, we will recall some notation and definitions from Chapter 1 that will be used throughout this section. Let $N \in \mathbb{N}$, $\phi : \mathbb{R}^* \to \mathbb{R}$, a, and $k^2 = \phi''(a)$ be defined as in definitions 1.15, 1.10, 1.11 (see pages 11 and 10). Let $\Lambda = \{(\mathbf{p}, \mathbf{q}) \in \mathbb{R}^N \times \mathbb{R}^N : q_i < q_{i+1} \text{ for all } i = 1, \ldots, N-1\}$. Let $\Phi : \Lambda \to \mathbb{R}^N \times \mathbb{R}^N$ be given by

$$\Phi(\mathbf{X}) = \Phi(\mathbf{p}, \mathbf{q}) = \begin{pmatrix} \phi'(q_2 - q_1) \\ \vdots \\ \phi'(q_{j+1} - q_j) - \phi'(q_j - q_{j-1}) \\ \vdots \\ -\phi'(q_N - q_{N-1}) \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{5.1}$$

where $j = 2, \ldots, N-1$. It is easy to see that Φ is locally Lipschitz on Λ. In agreement with the previous derivations, the memory kernel will be $\theta(t) = \frac{J_1(2kt)}{kt}$, however the proofs also go through if one considers functions of the form $\theta_T(t) = ar^{\left(\frac{t}{T_c}\right)^2}\theta(t)$, which will be of interest in the next chapter (See definition 6.10 on page 127 for details about θ_T). It will be convenient to have a matrix version of θ defined as $\Theta(t) = \operatorname{diag}(\underbrace{\theta(t), 0, \ldots, 0, \theta(t)}_{\text{associated to } p}, \underbrace{0, \ldots, 0}_{\text{associated to } q})$. Again the same following proofs will also go through if one replaces θ with θ_T.

5.1 Local Existence

5.1.1 Non-Markovian System

Lemma 5.1. *Let $f_L, f_R : \mathbb{R}^+ \to \mathbb{R}$ be continuous functions. Then there exists an $\epsilon > 0$ and a function $\mathbf{X} = (\mathbf{p}, \mathbf{q}) : [0, \epsilon) \to \Lambda$ satisfying the system of integro-differential equations*

$$\frac{dp_1}{dt} = \phi'(q_2 - q_1) - k^2 \int_0^t \theta(t-s) p_1(s) ds + k^2 f_L(t), \tag{5.2}$$

$$\frac{dp_j}{dt} = \phi'(q_{j+1} - q_j) - \phi'(q_j - q_{j-1}), \qquad \textit{for } j = 2, \dots, N-1, \tag{5.3}$$

$$\frac{dp_N}{dt} = -\phi'(q_N - q_{N-1}) - k^2 \int_0^t \theta(t-s) p_N(s) ds + k^2 f_R(t), \tag{5.4}$$

$$\frac{dq_j}{dt} = p_j, \qquad \textit{for } j = 1, \dots, N, \tag{5.5}$$

with initial conditions $\mathbf{X}(0) = (\mathbf{p}(0), \mathbf{q}(0)) = (\mathbf{p}_0, \mathbf{q}_0) \in \Lambda$.

Proof. The proof is the classical fixed point approach, however, it will behoove us to change notation a bit. Note that the system can be written as

$$\frac{d\,\mathbf{X}}{dt} = \Phi(\mathbf{X}) + \int_0^t \Theta(t-s)\,\mathbf{X}(s) ds + \mathbf{F}(s),$$

where $\mathbf{F}(s) = (\underbrace{f_L(s), 0 \dots, 0, f_R(s)}_{\mathbf{p}}, \underbrace{0 \dots, 0}_{\mathbf{q}})^t$. Fix $\mathbf{x}_0 = (\mathbf{p}_0, \mathbf{q}_0) \in \Lambda$, and choose $a > 0$ such that $B_a(\mathbf{x}_0) \subset \Lambda$. Fix $\epsilon > 0$, define $C = \mathcal{C}\left([0, \epsilon], \overline{B_a(\mathbf{x}_0)}\right)$ and equip it with the sup norm. Define the operator $\Gamma : C \to C$ by

$$(\Gamma\eta)(t) = \mathbf{x}_0 + \int_0^t \left[\Phi\left(\eta(s)\right) + \Theta * \eta(s) + \mathbf{F}(s)\right] ds.$$

For convenience set$M_{\mathbf{x}_0} = \max_{(y,s) \in \overline{B_a(\mathbf{x}_0)} \times [0,\epsilon]} (|\Phi(y)|, ||\Theta||_\infty |y|, |f(s)|)$. We need to check that Γ is a well defined map. This amounts to showing that $\Gamma\eta$ is continuous and $(\Gamma\eta)(t) \in \overline{B_a(\mathbf{x}_0)}$ whenever $t \in [0, \epsilon]$. Continuity is automatic by assumptions on Φ, Θ, and $\mathbf{F}$. To see that $(\Gamma\eta)(t) \in \overline{B_a(\mathbf{x}_0)}$ choose $t \leq \epsilon$. Then we see

$$
\begin{aligned}
&|(\Gamma\eta)(t) - \mathbf{x}_0| = \left| \int_0^t \left[\Phi(\eta(s)) + \Theta * \eta(s) + \mathbf{F}(s)\right] ds \right| \\
&\leq \int_0^t ||\Phi(\eta(s)) + \Theta * \eta(s) + \mathbf{F}(s)| \, ds \\
&\leq M_{\mathbf{x}_0} \int_0^t [1 + \epsilon + 1] \, ds \\
&\leq M_{\mathbf{x}_0}(\epsilon^2 + 2\epsilon),
\end{aligned}
$$

Now redefine ϵ so that $\epsilon^2 + 2\epsilon \frac{a}{M_{\mathbf{x}_0}}$. Doing so then gives

$$
|(\Gamma\eta)(t) - \mathbf{x}_0| < a,
$$

establishing that $(\Gamma\eta)(t) \in B_a(\mathbf{x}_0)$. At this point we want to show that Γ is a contraction after possibly further shrinking ϵ. Let $L_{\mathbf{x}_0}$ be the Local Lipschitz constant of Φ restricted to $\overline{B_a(\mathbf{x}_0)}$ and choose $\eta_1, \eta_2 \in C$. Then the difference

$$
\begin{aligned}
&|\Gamma\eta_1 - \Gamma\eta_2| \\
&\int_0^t [|\Phi(\eta_1(s)) - \Phi(\eta_2(s))| + |\Theta * (\eta_1 - \eta_2)(s)| \;] \, ds \\
&\int_0^\epsilon [L_{x_0}|\eta_1(s) - \eta_2(s)| + \epsilon||\Theta||_\infty ||\eta_1 - \eta_2||_\infty] \, ds \\
&\leq C_{\mathbf{x}_0}(\epsilon + \epsilon^2)||\eta_1 + \eta_2||_\infty.
\end{aligned}
$$

By choosing further $\epsilon + \epsilon^2 < \frac{1}{C_{\mathbf{x}_0}}$ we see that Γ is a contraction on C. Applying the Banach fixed point theorem now proves the lemma. $\square$

We will also need the following lemma to eventually prove global existence.

Lemma 5.2. *Let $f_L, f_R : \mathbb{R}^+ \to \mathbb{R}$ be continuous functions. Suppose that $\mathbf{X} = (\mathbf{p}, \mathbf{q}) : [0, t] \to \Lambda$ is the unique solution to the system of integro-differential equations of Lemma*

5.1 with $\mathbf{X}(0) = \mathbf{x}_0$ *on* $[0,t]$*. Then there exists and* $\epsilon > 0$ *such that* $\mathbf{X} : [0, t+\epsilon] \to \Lambda$ *is the unique solution to the system of integro-differential equations of Lemma 5.1 on* $[0, t+\epsilon]$*.*

Proof. Set $\mathbf{X}(t) = \mathbf{x}_t$. Choose $\epsilon, a > 0$ and define $C = \mathcal{C}\left([t, t+\epsilon], B_a(\mathbf{x}_t)\right)$. Further set $D = [t, t+\epsilon] \times \overline{B_a(\mathbf{x}_t)}$, and $M_{\mathbf{x}_t} = \max\limits_{(s,y)\in D} \left(|\Phi(y)|, ||\Theta||_\infty |y|, |f(s)|, ||\Theta||_\infty || \mathbf{X} ||_{L^\infty[0,t]}\right)$. Again let $L_{\mathbf{x}_t}$ be the local Lipschitz constant of Φ restricted to $\overline{B_a(\mathbf{x}_t)}$. Define the operator $\Gamma : C \to C$ by

$$(\Gamma\eta)(t+s) = \mathbf{x}_t + \int\limits_t^{t+s} \left[\Phi(\eta(\tau)) + \int_0^t \Theta(\tau-\sigma)\,\mathbf{X}(\sigma) d\sigma + \int_t^\tau \Theta(\tau-\sigma)\eta(\sigma) d\sigma + \mathbf{F}(\tau)\right] d\tau.$$

Continuity of $\Gamma\eta$ is again automatic. Now fix $\eta \in C$, then we find that

$$\begin{aligned}
&|(\Gamma\eta)(t+s) - \mathbf{x}_t| \\
&\le \int\limits_t^{t+s} \left[|\Phi(\eta(\tau))| + \int_0^t |\Theta(\tau-\sigma)\,\mathbf{X}(\sigma)| d\sigma + \int_t^\tau |\Theta(\tau-\sigma)\eta(\sigma)| d\sigma + |\mathbf{F}(\tau)|\right] d\tau \\
&\le \int\limits_t^{t+\epsilon} [M_{\mathbf{x}_t} + tM_{\mathbf{x}_t} + \epsilon M_{\mathbf{x}_t} + M_{\mathbf{x}_t}] \\
&\le M_{\mathbf{x}_t}\left(\epsilon + t\epsilon + \epsilon^2 + \epsilon\right) \\
&\le M_{\mathbf{x}_t}(\epsilon)(2 + t + \epsilon).
\end{aligned}$$

Now reselect ϵ so that $(\epsilon)(2+t+\epsilon) < \frac{a}{M_{\mathbf{x}_t}}$. This makes Γ a well defined map. To see now that Γ is a contraction fix $\eta_1, \eta_2 \in C$ and note that

$$\begin{aligned}
&|(\Gamma\eta_1)(s) - (\Gamma\eta_2)(s)| \\
&\le \int\limits_t^{t+\epsilon} \left[|\Phi(\eta_1(\tau)) - \Phi(\eta_2(\tau))| + \int_t^\tau |\Theta(\tau-\sigma)| \eta_1(\sigma) - \eta_2(\sigma)| d\sigma\right] d\tau \\
&\le \epsilon L_{\mathbf{x}_t} ||\eta_1 - \eta_2||_\infty + \epsilon^2 ||\Theta||_\infty ||\eta_1 - \theta_2||_\infty \\
&\le C(\epsilon + \epsilon^2) ||\eta_1 - \eta_2||_\infty.
\end{aligned}$$

Further choosing $\epsilon + \epsilon^2 < \frac{1}{C}$ makes Γ a contraction. Applying the Banach fixed point theorem and noting that $\mathbf{X}$ was already assumed to solve the desired system of IDE's on $[0, t]$ proves the lemma. $\square$

5.1.2 The Markovian Approximation

The global existence of the solution to the Markovian approximation is noted without proof in [28]. For completeness a proof of this fact is presented in this chapter. Here we prove that for any initial data laying in Λ, there exists a stopping time τ_Λ and a stopped process $X_t^{\tau_\Lambda}$ which is the unique solution to the Markovian approximation of the Lennard-Jones system whenever $t < \tau_\Lambda$.

Lemma 5.3. *Let B^L and B^R be two independent Weiner processes on $\mathbb{R}$. Then for any $(\mathbf{p}(0), \mathbf{q}(0)) = (\mathbf{p}_0, \mathbf{q}_0) \in \Lambda$ there exists a stopping time τ_Λ, such that the stopped process $\mathbf{X}_t^{\tau_\Lambda} = (\mathbf{p}_t^{\tau_\Lambda}, \mathbf{q}_t^{\tau_\Lambda})$ is a solution to the system of SDE's*

$$dp_1 = \left[\phi'(q_2 - q_1) - k^2 p_1\right] dt + k^2\sqrt{\beta_L} dB_t^L, \tag{5.6}$$
$$dp_j = \left[\phi'(q_{j+1} - q_j) - \phi'(q_j - q_{j-1})\right] dt, \text{ for } j = 2, \ldots, N-1, \tag{5.7}$$
$$dp_N = \left[-\phi'(q_N - q_{N-1}) - k^2 P_N\right] dt + k^2\sqrt{\beta_R} dB_t^R, \tag{5.8}$$
$$dq_j = p_j dt, \text{ for } j = 1, \ldots, N, \tag{5.9}$$

on $[0, \tau_\Lambda)$.

Proof. Note that we may write the above system of SDE's more compactly as

$$d\,\mathbf{X}_t = [\Phi(\mathbf{X}_t) + B\,\mathbf{X}_t]\,dt + \sigma dB_t$$

where $B, \sigma \in M_{2N}(\mathbb{R})$. Set $f(y) = \Phi(y) + By$, and note that f is locally Lipschitz on Λ. Fix $\mathbf{x}_0 = (\mathbf{p}_0, \mathbf{q}_0) \in \Lambda$. Let $F_n \subseteq \Lambda$ be compact, connected neighborhoods of $\mathbf{x}_0$, $\mathbf{x}_0 \in F_1$, $F_j \subseteq F_{j+1}$, and $\bigcup_{n\in\mathbb{N}} F_n = \Lambda$. Define now $f_N : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$ by $f_n(y) = f(y)\psi_n(y)$ where $\psi_n \in C_0^\infty(\mathbb{R}^{2N})$ with $\psi_n(y) = 1$ for all $y \in F_n$. Then from [33] we know that the associated system of SDE's

$$d\mathbf{X}_t^n = f_n(\mathbf{X}_t^n)dt + \sigma dB_t$$

has solution $\mathbf{X}_t^n$. Now let $\tau_{il} = \inf\{t \in \mathbb{R}^+ : \mathbf{X}_t^i \notin F_l^\circ\}$. For all $i, j \geq l$ almost surely $\tau_{il} = \tau_{jl}$ and the stopped processes $\mathbf{X}_t^{\tau_{il}} = \mathbf{X}_t^{\tau_{jl}}$ almost surely. Now let $\tau_\Lambda = \sup_l \tau_{ll}$. Then define for $t \in [0, \tau)$ $\mathbf{X}_t = \mathbf{X}_t^{\tau_{ll}}$ for $t < \tau_{ll}$. Then by construction, the stopped process $\mathbf{X}_t^\Lambda$ is a stochastic process, not depending on F, depending on Λ satisfying the SDE's of 5.3 on $[0, \tau_\Lambda)$ with initial conditions $\mathbf{x}_0$. $\square$

To prove global existence in time for the above system it suffices to prove that $\tau_\Lambda = \infty$ almost surely.

5.2 Global Existence

5.2.1 Non-Markov System

Theorem 5.4. *For any $\mathbf{x}_0 = (\mathbf{p}_0, \mathbf{q}_0) \in \Lambda$ there exists a global in time solution to the system of integro-differential equations of lemma 5.1 from page 78 with initial conditions $\mathbf{x}_0$.*

In order to prove this theorem, we will need a Gronwall type lemma.

Lemma 5.5. *Suppose that there exist continuous functions $u(t), A(t)$, $u(t) \geq 0$ for all $t \in \mathbb{R}^+$ and a $c > 0$ such that*

$$u(t) \leq A(t) + c\int_0^t \left[u(s) + t\int_0^s u(\tau)d\tau\right] ds. \tag{5.10}$$

Then there exists continuous function $\alpha(t), \beta(t)$ depending only on $A(t)$ such that

$$u(t) \leq A(t) + \alpha(t) + \beta(t). \tag{5.11}$$

Proof. Set $w(t) = \int_0^t \int_0^s u(\tau)d\tau ds$. Then we have that

$$\begin{aligned}
w''(t) &\le A(t) + cw'(t) + ctw(t) \\
\left(e^{-ct}w'(t)\right)' &\le A_1(t) + ctw(t)e^{-ct} \\
\left(e^{-ct}w'(t)\right)' &\le A_1(t) + ctw(t).
\end{aligned}$$

Now $ctw(t)) = \frac{c}{2}(t^2w(t))' - t^2w'(t)$. Note that $w'(t) = \int_0^t u(s)ds \ge 0$ for all $t \in \mathbb{R}^+$. Thus $ctw(t) \le \frac{c}{2}(t^2w(t))'$. Using this we find that

$$\begin{aligned}
\left(e^{-ct}w'(t)\right)' &\le A_1(t) + \frac{c}{2}(t^2w(t))' \\
w'(t) &\le A_2(t) + \frac{ct^2e^{ct}}{2}w(t) \\
w(t) &\le A_3(t) + \int_0^t \frac{cs^2e^{cs}}{2}w(s)ds.
\end{aligned}$$

By Gronwall's inequality [19] there exists continuous functions $\alpha(t)$ such that $w(t) \le \alpha(t)$ for all $t \in \mathbb{R}^+$. Then note that $w'(t) \le A_2(t) + \frac{ct^2e^{ct}}{2}w(t)$ implies there exists a continuous function $\beta(t)$ such that $w'(t) \le \beta(t)$ for all $t \in \mathbb{R}^+$. Thus

$$u(t) = w''(t) \le A(t) + c\beta(t) + ct\alpha(t),$$

proving the lemma. $\square$

Proof: Theorem 5.4. Fix $\mathbf{x}_0 = (\mathbf{p}_0, \mathbf{q}_0)) \in \Lambda$. Let $\Lambda \to \mathbb{R}$ be given by

$$H(\mathbf{p}, \mathbf{q}) = \sum_{j=1}^{N} \frac{p_j^2}{2} + \sum_{j=2}^{N-1} \phi(q_{j+1} - q_j) + \phi'(q_j - q_{j-1}) + C,$$

where $C = (2N-2)\phi(a)$ so that H is non-negative. Let $(\mathbf{p}_t, \mathbf{q}_t) : [0, T) \to \Lambda$ be a maximally extended solution of the system of equations of lemma 5.1 on page 78 with initial conditions $\mathbf{p}_0, \mathbf{q}_0$. Then $T = \inf\{t \in \mathbb{R}^+ : H(\mathbf{p}_t, \mathbf{q}_t) = \infty\}$, since if $\lim_{t\to T} H(\mathbf{p}(t), \mathbf{q}(t)) = \infty$, then for some j either some $\lim_{t\to T} p_j(t) = \infty$, or some $\lim_{t\to T} q_j(t) = \infty$, implying that $\lim_{t\to T} p_j(t) = \infty$, or that some $\lim_{t\to T} q_j(t) = \lim_{t\to T} q_{j+1}(t)$, and conversely if some $\lim_{t\to T} p_j(t) = \infty$, or some $\lim_{t\to T} q_j(t) = \infty$, implying that $\lim_{t\to T} p_j(t) = \infty$, or that some $\lim_{t\to T} q_j(t) = \lim_{t\to T} q_{j+1}(t)$, then $\lim_{t\to T} H(p(t), q(t)) = \infty$. The strategy of this proof will be to show that $T = \infty$. Note that we may write

$$
\begin{aligned}
&H(\mathbf{p}(t), \mathbf{q}(t)) \\
&= H(\mathbf{p}_0, \mathbf{q}_0) + \int_0^t (DH)(\mathbf{p}(s), \mathbf{q}(s))ds \\
&= H(\mathbf{p}_0, \mathbf{q}_0) + \int_0^t \nabla H(\mathbf{p}(s), \mathbf{q}(s)) \left(\dot{\mathbf{p}}(s), \dot{\mathbf{q}}(s)\right)^t ds \\
&= H(\mathbf{p}_0, \mathbf{q}_0) + \int_0^t \left[p_1(s)\left[\phi'(q_2(s) - q_1(s)) - k^2 \int_0^s \theta(s-\tau)p_1(\tau)d\tau + k^2 f_L(s)\right]\right. \\
&\qquad + \sum_{j=2}^{N-1} p_j(s)\left[\phi'(q_{j+1}(s) - q_j(s)) - \phi'(q_j(s) - q_{j-1}(s))\right] \\
&\qquad + p_N(s)\left[-\phi'(q_N(s) - q_{N-1}(s)) - k^2 \int_0^s \theta(s-\tau)p_N(\tau)d\tau + k^2 f_R(s)\right] \\
&\qquad - \phi'(q_2(s) - q_1(s))p_1(s) \\
&\qquad + \sum_{j=2}^{N-1} (-1)\left[\phi'(q_{j+1}(s) - q_j(s)) - \phi'(q_j(s) - q_{j-1}(s))\right] p_j(s) \\
&\qquad \left. + \phi'(q_N(s) - q_{N-1}(s))p_N(s)\right] ds \\
&= H(p_0, q_0) + \int_0^t \left[-k^2 p_1(s) \int_0^s \theta(s-\tau)p_1(\tau)d\tau + k^2 p_1(s) f_L(s)\right. \\
&\qquad \left. - k^2 p_N(s) \int_0^s \theta(s-\tau)p_N(\tau)d\tau + k^2 p_N(s) f_R(s)\right] ds.
\end{aligned}
$$

This allows us to compute the estimate

$$
\begin{aligned}
|H(\mathbf{p}(t), \mathbf{q}(t))| = |H(\mathbf{p}_0, \mathbf{q}_0)| + \int_0^t \left[\left|k^2 p_1(s) \int_0^s \theta(s-\tau)p_1(\tau)d\tau\right| + \left|k^2 p_1(s) f_L(s)\right|\right. \\
\left. \left|k^2 p_N(s) \int_0^s \theta(s-\tau)p_N(\tau)d\tau\right| + \left|k^2 p_N(s) f_R(s)\right|\right] ds.
\end{aligned}
$$

Young's inequality [19] gives

$$
\begin{aligned}
&|H(\mathbf{p}(t),\mathbf{q}(t))| \\
&= |H(\mathbf{p}_0,\mathbf{q}_0)| + \int_0^t \left[\frac{k^2}{2}p_1^2(s) + \frac{k^2}{2}\left|\int_0^s \theta(s-\tau)p_1(\tau)d\tau\right|^2 + \frac{k^2}{2}p_1^2(s) + \frac{k^2}{2}f_L^2(s)\right. \\
&\qquad \left.\frac{k^2}{2}p_N^2(s) + \frac{k^2}{2}\left|\int_0^s \theta(s-\tau)p_N(\tau)d\tau\right|^2 + \frac{k^2}{2}p_N^2(s) + \frac{k^2}{2}f_R^2(s)\right] ds \\
&\le |H(\mathbf{p}_0,\mathbf{q}_0)| + \int_0^t \left[k^2 p_1^s(s) + \frac{k^2}{2}\left[\int_0^s |p_1(\tau)|d\tau\right]^2 + \frac{k^2}{2}f_L^2(s)\right. \\
&\qquad \left.k^2 p_N^s(s) + \frac{k^2}{2}\left[\int_0^s |p_N(\tau)|d\tau\right]^2 + \frac{k^2}{2}f_R^2(s)\right] ds \\
&\le |H(\mathbf{p}_0,\mathbf{q}_0)| + \int_0^t \left[k^2 p_1^s(s) + \frac{k^2}{2}t\left[\int_0^s |p_1(\tau)|^2 d\tau\right] + \frac{k^2}{2}f_L^2(s)\right. \\
&\qquad \left.k^2 p_N^s(s) + \frac{k^2}{2}t\left[\int_0^s |p_N(\tau)|^2 d\tau\right] + \frac{k^2}{2}f_R^2(s)\right] ds \\
&\le |H(\mathbf{p}_0,\mathbf{q}_0)| + \int_0^t \left[\frac{k^2}{2}\left(f_L^2(s) + f_R^2(s)\right) + H(\mathbf{p}(s),\mathbf{q}(s)) + t\int_0^s H(\mathbf{p}(\tau),\mathbf{q}(\tau))d\tau\right] ds
\end{aligned}
$$

Now applying the lemma 5.5 from page 82 we have that $H(\mathbf{p}(t),\mathbf{q}(t)) < \infty$ for all $t \in \mathbb{R}^+$, concluding the proof. □

5.2.2 The Markovian Approximation

Theorem 5.6. *The stopping time $\tau_\Lambda = \infty$ almost surely.*

Proof. For ease of notation, let the stopped process of lemma 5.3 from page 81 be denoted by $\mathbf{X}_t = (\mathbf{p}_t, \mathbf{q}_t)$. Suppose that $\mathbf{X}_0 = (\mathbf{q}_0, \mathbf{p}_0) \in \Lambda$ is deterministic. The infinitesimal generator [46] for the system of SDE's of lemma 5.3 in Λ is

$$L = \left[\phi'(q_2 - q_1) - k^2 p_1\right]\partial_{p_1} + \sum_{j=2}^{N-1}\left[\phi'(q_{j+1} - q_j) - \phi'(q_j - q_{j-1})\right]\partial_{p_j}$$

$$+\left[-\phi'(q_N - q_{N-1}) - k^2 p_N\right]\partial_{p_N} + \sum_{j=1}^{N} p_i \partial_{q_i} + \frac{1}{2}k^4\beta_L\partial^2_{p_1} + \frac{1}{2}k^4\beta_R\partial^2_{p_N}.$$

Define the Hamiltonian $H : \Lambda \to \mathbb{R}$ by

$$H(\mathbf{p},\mathbf{q}) = \sum_{j=1}^{N}\frac{p_j^2}{2} + \sum_{j=2}^{N-1}\phi(q_{j+1}-\phi_j) + \phi(q_j - q_{j-1}) + C.$$

where $C = (2N-2)\phi(a)$ so that H is non-negative. Fix $M \in \mathbb{R}$. Then let $D = H^{-1}([0,M])$, and $D_m = D \cap \overline{B_m(0)}$. Each D_m is compact by construction. Now define $H_n = H(\mathbf{p},\mathbf{q})\chi_m(\mathbf{p},\mathbf{q})$ where χ is a (compactly supported) smooth bump function with $\chi(\mathbf{p},\mathbf{q}) = 1$ whenever $(\mathbf{p},\mathbf{q}) \in D_n$ and $(\mathbf{p},\mathbf{q}) \leq 1$ otherwise. Define the stopping time $\tau_{D_m} = \inf\{s \in \mathbb{R}^+ : \mathbf{X}(s) \notin D_m\}$, and set $\tau_m = t \wedge \tau_{D_m}$. Then for each automatically $\mathbb{E}\left[\tau_m\right] < \infty$. Since H_m is a smooth compactly supported bump function we may apply Dynkin's formula [46]:

$$\mathbb{E}\left[H_m(\mathbf{p}_{\tau_m},\mathbf{q}_{\tau_m})\right] = H_n(\mathbf{p}_0,\mathbf{q}_0) + \mathbb{E}\left[\int_0^{\tau_m}(LH_n)(\mathbf{p}(s),\mathbf{q}(s))ds\right],$$

where $\mathbf{p}_{\tau_m} = \mathbf{p}(\tau_m)$ and $\mathbf{q}_{\tau_m} = \mathbf{q}(\tau_m)$. Now on D_N

$$\begin{aligned}
(LH)(\mathbf{p},\mathbf{q}) = &\left[\phi'(q_2-q_1) - k^2p_1\right]p_1 \\
&+ \sum_{j=2}^{N-1}\left[\phi'(q_{j+1}-q_j) - \phi'(q_j - q_{j-1})\right]p_j \\
&+ \left[-\phi'(q_N - q_{N-1}) - k^2p_N\right]p_N \\
&- p_1\phi'(q_2 - q_1) \\
&+ \sum_{j=2}^{N-1} p_j\left[-\phi'(q_{j+1}-q_j) + \phi'(q_j - q_{j-1})\right] \\
&+ p_N\phi'(q_N - q_{N-1}) \\
&+ \frac{1}{2}k^4\beta_L + \frac{1}{2}k^4\beta_R \\
= &-k^2p_1^2 - k^2p_N^2 + \frac{1}{2}k^4(\beta_L+\beta_R).
\end{aligned}$$

So Dynkin's formula takes the form

$$\mathbb{E}\left[H_m(\mathbf{p}(\tau_m), \mathbf{q}(\tau_m))\right] = H_n(\mathbf{p}_0, \mathbf{q}_0) + \mathbb{E}\left[\int_0^{\tau_m} \left[-k^2 p_1^2 - k^2 p_N^2 + \frac{1}{2}k^4(\beta_t + \beta_R)\right]\right].$$

In particular this shows that there is a constant C, depending only on k, β_L and β_R

$$\mathbb{E}\left[H_m(\mathbf{p}(\tau_m), \mathbf{q}(\tau_m))\right] \leq H(\mathbf{p}_0, \mathbf{q}_0) + C\mathbb{E}\left[\tau_m\right].$$

Now define the stopped process $(\mathbf{p}_t^{D_m}, \mathbf{q}_t^{D_m}) = (\mathbf{p}_{\tau_m}, \mathbf{q}_{\tau_m})$ (remember $\tau_m = t \wedge \tau_{D_m}$. Then the previous calculation shows that

$$\mathbb{E}\left[H_m(\mathbf{p}_t^{D_m}, \mathbf{q}_t^{D_m})\right] \leq H(\mathbf{p}_0, \mathbf{q}_0) + C\mathbb{E}\left[\tau_m\right] \leq H(\mathbf{p}_0, \mathbf{q}_0) + Ct.$$

Note that the right hand side does not depend on M or m. So by passing m and then M to infinity, we establish

$$\mathbb{E}\left[H(\mathbf{p}_t, \mathbf{q}_t)\right] \leq H(\mathbf{p}_0, \mathbf{q}_0) + Ct.$$

Thus $H(\mathbf{p}_t, \mathbf{q}_t) < \infty$ for all $t \in \mathbb{R}^+$ almost surely, and so we can conclude that $\tau_\Lambda < \infty$ almost surely. □

Chapter 6

Simulating the Dynamics

Chapter 5 establishes the existence of GLE's whose non-autonomous part is continuous in time; we now turn out attention to simulating such systems. When the noise is assumed to be stationary, Kolmogorov's continuity theorem [46] shows that almost every sample path is continuous. For the non-stationary case it will be shown the noise is almost surely continuous.

Not only do we want to understand the effect of memory on observables of the system, we also want to understand to what degree the non-stationarity affects observables, and, in particular, how the scaling of conductivity presented in definition 1.8 is affected by non-stationarity of the noise. This means that we will need to simulate GLE's representing both the exact dynamics where the noise is not stationary, and ones in which we assume the noise is stationary and satisfies the fluctuation dissipation theorem. The GLE's arising with non-stationary noise will be called the non-stationary GLE's, while the GLE's arising from enforcing stationarity and the fluctuation dissipation theorem will be called the stationary GLE's. For both cases, to simulate the GLE's, convolutions must be performed at each time step. Naively one would expect an $O(N^2)$ operations would be needed, where N is the total number of time steps of the simulation. Since $N \approx 10^7$, simulating the systems becomes very expensive. Fortunately, one can get around this by using a sum of exponentials approximation of the memory kernel, which allows computation of convolutions with effectively $O(N \log N)$ operations.

6.1 Fast Convolution and the Sum of Exponential Approximation

6.1.1 Fast and Efficient Convolutions of Sums of Exponentials

In this section we follow [32].

Let $f : [0, \infty) \to \mathbb{R}$ be continuous. Suppose one wants to evaluate the function

$$I(t) = \int_0^t \sum_{j=1}^{M} w_j e^{\gamma_j (t-s)} f(s) ds \tag{6.1}$$

on the uniformly spaced grid $\Delta t\mathbb{N}$, where $\Delta t > 0$. Let $I_n = I(n\Delta t)$, and

$$C_j(n) = \int_0^{n\Delta t} w_j e^{\gamma_j (n\Delta t - s)} ds. \tag{6.2}$$

Then note that

$$\begin{aligned}
C_j(n) &= \int_0^{n\Delta t} w_j e^{\gamma_j (n\Delta t - s)} f(s) ds \\
&= \int_0^{(n-1)\Delta t} w_j e^{\gamma_j ((n-1)\Delta t + \Delta t - s)} f(s) ds + \int_{(n-1)\Delta t}^{n\Delta t} w_j e^{\gamma_j (n\Delta t - s)} f(s) ds \\
&= e^{\gamma_j \Delta t} C_j(n-1) + \int_{(n-1)\Delta t}^{n\Delta t} w_j e^{\gamma_j (n\Delta t - s)} f(s) ds.
\end{aligned}$$

Since $I_n = \sum_{j=1}^{M} C_j(n)$ for all $n \in \mathbb{N}$, to evaluate I_n, we first need to compute each $C_j(n)$ which only takes $O(1)$ operations, then sum all M of them to arrive at the result. Moreover, only $C_j(n-1)$ is needed to compute $C_j(n)$, giving an $O(M)$ memory requirement. It turns out that one can also use this technique to efficiently evaluate $I(n\Delta t + \delta)$ for $0 \leq \delta \leq \Delta t$. With $C_j(n)$ defined as before note that

$$\begin{aligned}
&\int_0^{n\Delta t+\delta} w_j e^{\gamma_j(n\Delta t+\delta-s)} f(s)ds \\
&= e^{\gamma_j\delta}\left[\int_0^{n\Delta t} w_j e^{\gamma_j(n\Delta t-s)} f(s)ds + \int_{n\Delta t}^{n\Delta t+\delta} w_j e^{\gamma_j(n\Delta t-s)} f(s)ds\right] \\
&= e^{\gamma_j\delta}\left[C_j(n) + \int_{n\Delta t}^{n\Delta t+\delta} w_j e^{\gamma_j(n\Delta t-s)} f(s)ds\right].
\end{aligned}$$

This establishes

$$I(n\Delta t + \delta) = \sum_{j=1}^{M} e^{\gamma_j\delta}\left[C_j(n) + \int_{n\Delta t}^{n\Delta t+\delta} w_j e^{\gamma_j(n\Delta t-s)} f(s)ds\right]. \tag{6.3}$$

This result allows computation of I at fractional time steps which is often required by numerical ODE schemes, e.g Runge-Kutta methods. The memory kernels we are interested in are not a sum of exponentials, however we can use the fast convolution technique by uniformly approximating the memory kernels by sums of exponentials.

6.1.2 Approximation by Sums of Exponentials

There are two variants of approximation of a function by sums of exponentials: the continuous version and the discrete version.

Definition 6.1. *Let $\theta : [0, T] \to \mathbb{R}$ and let $\epsilon > 0$. If there exists $M \in \mathbb{N}$ and $w_j, \gamma_j \in \mathbb{C}$, $j = 1, \ldots, M$ such that*

$$\left|\left|\theta(t) - \sum_{j=1}^{M} w_j e^{\gamma_j t}\right|\right|_{\infty}. \tag{6.4}$$

Then $\sum_{j=1}^{M} w_j e^{\gamma_j t}$ *is said to be a (continuous) sum of exponentials approximation of* θ *of order* ϵ*.*

Definition 6.2. *Suppose we have* $N \in \mathbb{N}$ *samples* $\{\theta_j \in \mathbb{R} : j = 0, \dots N\}$ *of some function* θ *at equally spaced points in time ranging from* 0 *to* T*. Let* $\epsilon > 0$*. Then the data samples* $\{\theta_j\}_{j=0}^{N}$ *is said to admit a (discrete) sum of exponential approximation if there exists* $M \in \mathbb{N}$ *and* $w_j, z_j \in \mathbb{C}$*,* $j = 1, \dots, M$ *such that*

$$\left|\theta_n - \sum_{j=1}^{M} w_j z_j^n\right| < \epsilon \quad n = 0, \dots, N. \tag{6.5}$$

A continuous sum of exponentials approximation immediately gives a discrete sum of exponentials approximation by restriction to a uniform grid. Similarly, a discrete sum of exponentials approximation gives rise to a continuous sum of exponentials approximation by the choice $\gamma_j = \frac{log(z_j)}{h}$, where h is the grid size of the discrete sum of exponentials approximation. The newly produced continuous sum of exponentials approximation however will in general have larger error than the discrete version which generated it. Upon reviewing the literature, it seems the sum of exponentials approximation is largely considered a settled matter. Beylkin and Monzón [5] introduce and provide some error analysis for efficient sum of exponential approximation. Unfortunately, direct application of their method was not practical for the purposes of this research. It requires the user to find roots of a particular polynomial in a "significant" region, which is not known a priori. In their paper, the polynomials are low enough degree where standard root finding algorithms are safe. In our case, this would involve finding the roots of a polynomial of degree on the order of thousands. Instead, we use the matrix pencil method developed by Sarkar and Pereira in [54] to generate discrete sums of exponential approximation.

Suppose that we have $N+1$ data samples $\{\theta_j \in \mathbb{R} : j = 0, \ldots, N\}$, where N is even, and that there is an $M \in \mathbb{N}$ and $z_j \neq 0, w_j \neq 0 \in \mathbb{C}$, $j = 1, \ldots, M$ such that

$$\begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_N \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_M \\ \vdots & \vdots & & \vdots \\ z_1^N & z_2^N & \cdots & z_M^N \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_M \end{bmatrix}, \tag{6.6}$$

where each z_j is distinct. Further, form the matrices

$$\Theta = \begin{bmatrix} \theta_0 & \theta_1 & \cdots & \theta_{N/2} \\ \theta_1 & \theta_2 & \cdots & \theta_{N/2+1} \\ \vdots & \vdots & & \vdots \\ \theta_{N/2} & \theta_{N/2+1} & \cdots & \theta_N \end{bmatrix}.$$

Let $U\Sigma V^*$ be the singular value decomposition of Θ. Fix a tolerance $\epsilon > 0$ and choose $M = \min\{j \in \mathbb{N} : \sigma_j < \epsilon\}$. We may now form the truncated partial SVD of Θ. Let $V' = [v_1 \ldots v_M]$ be the matrix of the first M right singular vectors of Θ. Set $\Theta'_j = U\Sigma' V_j'^*, j = 1, 2$ where V'_1 and V'_2 are obtained from V' by deleting the last and first row respectively. Additionally define the submatrices of Θ

$$\Theta_1 = \begin{bmatrix} \theta_0 & \theta_1 & \cdots & \theta_{N/2-1} \\ \theta_1 & \theta_2 & \cdots & \theta_{N/2} \\ \vdots & \vdots & & \vdots \\ \theta_{N/2} & \theta_{N/2+1} & \cdots & \theta_{N-1} \end{bmatrix}, \Theta_2 = \begin{bmatrix} \theta_1 & \theta_2 & \cdots & \theta_{N/2} \\ \theta_2 & \theta_3 & \cdots & \theta_{N/2+1} \\ \vdots & \vdots & & \vdots \\ \theta_{N/2+1} & \theta_{N/2} & \cdots & \theta_N \end{bmatrix}.$$

Note that Θ_1 the the submatrix formed by deleting the last column of Θ, and Θ_2 is the submatrix formed by deleting the first column of Θ. Then Θ_1 and Θ_2 satisfy the matrix equations

$$\Theta_1 = Z_1 R Z_2, \tag{6.7}$$
$$\Theta_2 = Z_1 R Z_0 Z_2, \tag{6.8}$$

where

$$Z_1 = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_M \\ \vdots & \vdots & & \vdots \\ z_1^{N/2} & z_2^{N/2} & \cdots & z_M^{N/2} \end{bmatrix}, \tag{6.9}$$

$$Z_2 = \begin{bmatrix} 1 & z_1 & \cdots & z_1^{N/2-1} \\ 1 & z_2 & \cdots & z_2^{N/2-1} \\ \vdots & \vdots & & \vdots \\ 1 & z_M & \cdots & z_M^{N/2-1} \end{bmatrix}, \tag{6.10}$$

$$Z_0 = \operatorname{diag}\left[z_1, z_2, \ldots, z_M\right], \tag{6.11}$$

$$W = \operatorname{diag}\left[w_1, w_2, \ldots, w_M\right], \tag{6.12}$$

$$||\Theta_j - \Theta_j'||_2 = O(\epsilon). \tag{6.13}$$

The matrices Z_1 and Z_2 are full rank since they are Vandermonde matrices with distinct z_j generating entries [62]. The matrices Z_0 and W are full rank since none of the diagonal entries are zero by assumption. The order comparison of equation (6.13) follows from

$$||\Theta_j - \Theta_j'||_2 = |||U\Sigma(\Pi_j V) - U\Sigma(\Pi_j V \Pi_M)||_2$$
$$||U\Sigma(\Pi_j V(1-\Pi_M))^*||_2 = ||U(\Sigma(1-\Pi_M)^*)^* V \Pi_j^*||_2 = O(\epsilon),$$

where Π_j are the projectors corresponding to deleting the first or last row, and Π_M of V are the projectors corresponding to deleting the last $(N/2 - M)$ columns of V. Let $\lambda \in \mathbb{C}$. The matrix pencil of Θ_1 and Θ_2 is by definition $\Theta_2 - \lambda\Theta_1$. The matrix pencil satisfies

$$\Theta_2 - \lambda\Theta_1 = Z_1 R\left[Z_0 - \lambda\right] Z_2. \tag{6.14}$$

An important observation of the matrix pencil method is that the matrix pencil of Θ_1 and Θ_2 has deficient rank if and only if $\lambda = z_j$ for some $j = 1, \ldots M$. Hence the nodes z_j are found by solving the generalized eigenvalue problem for the pair (Z_1, Z_2). However since Θ_1 has full rank, the generalized eigenvalue problem corresponds to an ordinary eigenvalue problem for the matrix $\Theta_1^\dagger \Theta_2$ where $\Theta_1^\dagger$ denotes the pseudoinverse. Solving the generalized eigenvalue problem for Z_1 and Z_2 could be expensive for large N. Instead, we solve the generalized eigenvalue problem for the pair (Θ_1', Θ_2') to arrive at an approximate generalized eigenvalue for Θ_1 and Θ_2, and hence an approximation of the z_j. This works as follows. Since U, Σ', Θ_1', and Θ_2' have full rank, λ is a generalized eigenvector of the pair (Θ_2, Θ_1) if and only if λ is an eigenvector of $(V_1'^*)^\dagger V_2'^*$. So if λ is an eigenvalue of $(V_1'^*)^\dagger V_2'^*$ with eigenvector v, then

$$||(\Theta_2 - \lambda\Theta_1)v|| = ||(\Theta_2' - \lambda\Theta_1')v|| + O(\epsilon) = O(\epsilon).$$

Thus λ is also an approximate generalized eigenvalue of the pair (Θ_1, Θ_2). In particular, by finding $z_1', \ldots, z_M'$ approximate eigenvectors of the pair (Θ_1, Θ_2) by this method, we then find that

$$\left|\left| \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_N \end{bmatrix} - \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_M \\ \vdots & \vdots & & \vdots \\ z_1^N & z_2^N & \cdots & z_M^N \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_M \end{bmatrix} \right|\right| = O(\epsilon).$$

This tells us that solving for approximate generalized eigenvalues produces errors on the same order as the chosen tolerance. Because $(V_1'^*)^\dagger V_2'^*$ is an $M \times M$ matrix, this process becomes much more computationally efficient than trying to solve the generalized eigenvalue problem for (Θ_1, Θ_2). Due to the bandlimited nature of the velocity memory kernel $\theta(t)$, this method of producing a sum of exponentials approximation is very efficient. With a final time of $T = 10^4$, when the memory kernel is sampled uniformly with a coarse time step of $\Delta t = 0.2$, a continuous sum of exponentials approximation with only 53 terms is produced in only a few minutes on the authors laptop and results in a infinity norm error bounded above by 8.3975×10^{-12} when evaluated on a finer grid with spacing $\Delta t = 0.001$.

6.2 Non-Stationary GLE

The non-stationary GLE's are

$$\ddot{u}_1 = \phi'(u_2 - u_1 + a) - k^2\theta(t)u_1(0) - k^2 \int_0^t \theta(t-s)\dot{u}_1(s)ds + k^2 F_L(t), \tag{6.15}$$

$$\ddot{u}_j = \phi'(u_{j+1} - u_j + a) - \phi'(u_j - u_{j-1} + a), \quad j = 2, \dots, N-1, \tag{6.16}$$

$$\ddot{u}_N = -\phi'(u_{N-1} - u_N + a) - k^2\theta(t)u_1(0) - k^2 \int_0^t \theta(t-s)\dot{u}_N(s)ds + k^2 F_R(t), \tag{6.17}$$

where ϕ is the confined Lennard Jones potential from definition 1.10 on page 10, a is the constant defined in 1.9 on page 9, $\theta(t) = J_1(2kt)/(kt)$ from lemma 4.8 on page 69, and F is the non stationary noise term defined by 4.4 on page 63. To calculate F, we derive an infinite system of ODE's with random initial conditions which reconstruct F.

6.2.1 Generating the Non-Stationary Noise

The following derivation is only performed for the left bath, but the derivation for the right bath is analogous and found by reindexing. From proposition 4.4 on page 63,

$$\tilde{F}(s) = \frac{1}{k^2} \sum_{j \le 0} \tilde{\beta}^{|j|+1}(s) f_j(s) = \sum_{j \le 0} \frac{\tilde{\beta}^{|j|+1}(s)}{k^2} \dot{u}_j(0) + \frac{s\tilde{\beta}^{|j|+1}(s)}{k^2} u_j(0). \tag{6.18}$$

Inverting back to time domain, we may write the noise term as

$$F(t) = \sum_{j \le 0} a_j(t)\dot{u}_j(0) + b_j(t)u_j(0), \tag{6.19}$$

where we use the following definitions:

Definition 6.3. *For all $j \leq 0$, the functions $a_j(t)$ and $b_j(t)$ are defined via their Laplace transforms $\tilde{a}_j(t)$ and $\tilde{b}_j(t)$ which are given by*

$$\tilde{a}_j(s) = \frac{\tilde{\beta}^{|j|+1}(s)}{k^2}, \tag{6.20}$$

$$\tilde{b}_j(s) = \frac{s\tilde{\beta}^{|j|+1}(s)}{k^2}. \tag{6.21}$$

An analogous definition holds for the right bath.

Lemma 6.1. *For all $j \leq 0$ the following hold:*

1. $a_j(0) = 0$.

2. $\dot{a}_j(t) = b_j(t)$.

3. $\dot{a}_j(0) = \delta_{0j}$.

Proof. Fix $j \leq 0$ throughout. For item (*1.*), the initial value theorem for Laplace transforms [10] gives

$$a_j(0) = \lim_{s\to\infty} \frac{s\tilde{\beta}^{|j|+1}(s)}{k^2} = \frac{1}{k^2} \lim_{s\to\infty} s \left[\frac{2k^2}{s^2 + 2k^2 + \sqrt{s^4 + 2k^2 + \sqrt{s^4 + 4k^2 s^2}}} \right]^{|j|+1} = 0$$

For item (*2.*), the Laplace transform os $\dot{a}_j(t)$ is given by $s\tilde{a}_j(s) - a_j(0)$. Since item (*1.*) of the lemma establishes $a_j(0) = 0$, we have that $\dot{a}_j(t)$ has Laplace transform $s\tilde{a}_j(s)$, which in turn satisfies

$$s\tilde{a}_j(s) = s\frac{\tilde{\beta}^{j+1}(s)}{k^2} = \tilde{b}_j(s).$$

Thus $\dot{a}_j(t) = b_j(t)$. Lastly, for item (*3.*) the initial value theorem for Laplace transforms [10]:

$$\dot{a}_j(0) = \frac{1}{k^2} \lim_{s\to\infty} ss \left[\frac{2k^2}{s^2 + 2k^2 + \sqrt{s^4 + 4k^2 s^2}} \right]^{|j|+1}.$$

For $j < 0$

$$\lim_{s\to\infty} ss \left[\frac{2k^2}{s^2 + 2k^2 + \sqrt{s^4 + 4k^2 s^2}} \right]^{|j|+1} = 0,$$

while for $j = 0$

$$\lim_{s\to\infty} ss \left[\frac{2k^2}{s^2 + 2k^2 + \sqrt{s^4 + 4k^2 s^2}} \right] = \frac{1}{k^2} \frac{2k^2}{2} = 1.$$

Hence $b_j(0) = \delta_{0j}$. □

We can now write down a set of ODE's for all but one of the a_j

Lemma 6.2. *For $j < 0$,*

$$\ddot{a}_j(t) = -\mathcal{L}(a_j)(t), \tag{6.22}$$

where $-\mathcal{L}(a_j) := k^2(a_{j-1} - 2a_j + a_{j+1})$.

Proof. Since $a_j(0) = \dot{a}_j(0) = 0$, proving the lemma amounts to proving that

$$s^2 \tilde{a}_j(s) = -\mathcal{L}(\tilde{a}_j)(s).$$

Computing the right hand side we find

$$\begin{aligned}
&- \mathcal{L}(\tilde{a}_j)(s) = k^2 \left(\tilde{a}_{j-1}(s) - 2\tilde{a}_j(s) + \tilde{a}_{j+1}(s)\right) \\
&= \left(\tilde{\beta}^{|j|+2}(s) - 2\tilde{\beta}^{|j|+1}(s) + \tilde{\beta}^{|j|}(s)\right) \\
&= \tilde{\beta}^{|j|}(s) \left(\tilde{\beta}^2(s) - 2\tilde{\beta}(s) + 1\right)
\end{aligned}$$

$$
\begin{aligned}
&= \tilde{\beta}^{|j|}(s)\left[\tilde{\beta}(s)-1\right]^2 \\
&= \tilde{\beta}^{|j|}(s)\left[\frac{s^2+2k^2-\sqrt{s^4+4k^2s^2}}{2k^2}-1\right] \\
&= \tilde{\beta}^{|j|}(s)\left[\frac{s^2-\sqrt{s^4+4k^2s^2}}{2k^2}\right] \\
&= \tilde{\beta}^{|j|}(s)\left[\frac{s^4-2s^2\sqrt{s^4+4k^2s^2}+s^4+4k^2s^2}{4k^4}\right] \\
&= \tilde{\beta}^{|j|}(s)\left[\frac{2s^4+4k^2s^2-2s^2\sqrt{s^4+4k^2s^2}}{4k^4}\right] \\
&= \tilde{\beta}^{|j|}(s)\left[\frac{s^4+2k^2s^2-s^2\sqrt{s^4+4k^2s^2}}{2k^4}\right] \\
&= \frac{s^2}{k^2}\tilde{\beta}^{|j|}(s)\left[\frac{s^2+2k^2-\sqrt{s^4+4k^2s^2}}{2k^2}\right] \\
&= s^2\frac{\tilde{\beta}^{|j|}(s)}{k^2}\tilde{\beta}(s) \\
&= s^2\frac{\tilde{\beta}^{|j|+1}(s)}{k^2} \\
&= s^2\tilde{a}_j(s).
\end{aligned}
$$

Transforming back to time domain gives the result. □

Lemma 6.3. *The function $a_0(t)$ satisfies*

$$
a_0(t) = \frac{2J_1(2kt)}{k^3t^2} - \frac{2J_0(2kt)}{k^2t}. \tag{6.23}
$$

Proof. From definition 1.24 on page 15, is is easy to see $\theta'(t) = -\beta(t)$. Since $a_0(t) = \frac{1}{k^2}\beta(t)$, we have that $a_0(t) = -\frac{1}{k^2}\theta'(t)$. From lemma 4.8 on page 69, $\theta(t) = \frac{J_1(2kt)}{kt}$, we see that

$$
\begin{aligned}
a_0(t) &= -\frac{1}{k^2}\theta'(t) \\
&= -\frac{1}{k^2}\frac{d}{dt}\left[\frac{J_1(2kt)}{kt}\right]
\end{aligned}
$$

$$= -\frac{1}{k^2}\left[\frac{ktJ_1'(2kt)(2k) - J_1(2kt)(k)}{k^2t^2}\right]$$
$$= -\frac{1}{k^2}\left[\frac{2k^2tJ_1'(2kt) - kJ_1(2kt)}{k^2t^2}\right].$$

Calculating the derivative, $J_1'(x) = J_0(x) - \dfrac{J_1(x)}{x}$. Using this we find

$$a_0(t) = -\frac{1}{k^2}\left[\frac{2k^2t\left(J_0(2kt) - \frac{J_1(2kt)}{2kt}\right) - kJ_1(2kt)}{k^2t^2}\right]$$
$$= -\frac{1}{k^2}\left[\frac{2k^2tJ_0(2kt) - kJ_1(2kt) - kJ_1(2kt)}{k^2t^2}\right]$$
$$= -\frac{1}{k^2}\left[\frac{2k^2tJ_0(2kt) - 2kJ_1(2kt)}{k^2t^2}\right]$$
$$= -\frac{1}{k^2}\left[\frac{2ktJ_0(2kt) - 2J_1(2kt)}{kt^2}\right]$$
$$= \frac{2J_1(2kt) - 2ktJ_0(2kt)}{k^3t^2}$$
$$= \frac{2J_1(2kt)}{k^3t^2} - \frac{2J_0(2kt)}{k^2t}.$$

$\square$

Theorem 6.4. *The noise terms F_L and F_R satisfy*

$$F_L(t) = \sum_{j=-\infty}^{0} a_j(t)\dot{u}_j(0) + \dot{a}_j(t)u_j(0), \tag{6.24}$$
$$F_R(t) = \sum_{j=N+1}^{\infty} a_j(t)\dot{u}_j(0) + \dot{a}_j(t)u_j(0), \tag{6.25}$$

where the a_j satisfy the following first order system

$$\dot{a}_j = k^2(a_{j-1} - 2a_j + a_{j+1}),\ \textit{for } j \le -1, \tag{6.26}$$
$$a_0(t) = \frac{2J_1(2kt)}{k^3t^2} - \frac{2J_0(2kt)}{k^2t}, \tag{6.27}$$
$$a_j = a_{N+1-j},\ \textit{for } j = N+1, \ldots, (N+1)+M, \tag{6.28}$$
$$b_j = \dot{a}_j,\ \textit{for } j = N+1, \ldots, (N+1)+M, \tag{6.29}$$

$$a_j(0) = 0, \ \mathit{for}\ j \leq 0, j \geq N+1, \tag{6.30}$$
$$\dot{a}_j(0) = \delta_{0j}\ \mathit{for}\ j \leq 0, j \geq N+1. \tag{6.31}$$

Proof. Combine equation 6.19, lemma 6.2, and lemma 6.3 from pages 95, 97, and 98, and analogously for the right bath. □

In operator form, the ODE's modeling the noise for an individual bath are of the form

$$\frac{d}{dt}\begin{bmatrix} b(t) \\ a(t) \end{bmatrix} = \begin{bmatrix} 0 & -\mathcal{L} \\ I & 0 \end{bmatrix}\begin{bmatrix} b(t) \\ a(t) \end{bmatrix} + a_0(t)\begin{bmatrix} 0 \\ \mathbf{e}_{-1} \end{bmatrix}, \tag{6.32}$$

with $a(0) = b(0) = 0$. Because of the zero initial conditions and the fact that the scaled discrete Laplace operator $\mathcal{L}$ is a bounded operator on $l^2(\mathbb{N}^-)$, the above system has global solutions in time in $l^2(\mathbb{N}^-) \times l^2(\mathbb{N}^-)$ given by

$$\int_0^t \exp\left((t-s)\begin{pmatrix} 0 & -\mathcal{L} \\ I & 0 \end{pmatrix}\right)\begin{pmatrix} 0 \\ \mathbf{e}_{-1} \end{pmatrix} k^2 a_0(s)ds. \tag{6.33}$$

To truncate this infinite set of ODE's to a finite system we must define appropriate boundary conditions for $\mathcal{L}$. The boundary condition at index -1 is Dirichlet, since $a_0(t)$ is known. For the other boundary we use an absorbing boundary condition. We now derive an absorbing boundary condition to truncate the ODE system corresponding ot the left noise in theorem 6.4. The process is nearly identical for the right noise. Fix $M < 0$. Since $\mathcal{L}$ is a discrete Laplace operator, we expect a to act as though it were a wave equation where the indexes are labeling a spatial discretization. In particular

$$\ddot{a}_M = k^2 \Delta x^2 \frac{a_{M-1} - 2a_N + a_{M+1}}{\Delta x^2},$$

where Δx is a fixed positive number representing the spacing of our virtual spatial discretization. The wave speed of the above equation is $k\Delta x$, which seemingly depends on the spatial discretization. Putting an absorbing boundary condition on the left boundary amounts to requiring that left-traveling transport equation with the same wave speed as the wave equation is satisfied at a_M:

$$\frac{\partial a_M}{\partial t} = k\Delta x \frac{\partial a_M}{\partial x}.$$

This is discretized as

$$\frac{\partial a_M}{\partial t} = k\Delta x \left(\frac{-a_{M-1} + a_M}{\Delta x} + O(\Delta x) \right) = k(a_M - a_{M-1}) + O(\Delta x^2).$$

Since Δx is arbitrary, we may pass it to zero and get the exact condition

$$\frac{da_M}{dt} = k(a_M - a_{M-1}).$$

Now we know that $b_M = \dot{a}_M$, so $b_M = ka_M - ka_{M-1}$. Substituting this into the equation for $\dot{b}_M$ gives

$$\dot{b}_M = k^2(a_{M-1} - 2a_M + a_{M+1}) = k^2 \left(a_M - \frac{b_M}{k} - 2a_M + a_{M+1} \right) = k^2 \left(-\frac{b_M}{k} - a_M + a_{M+1} \right)$$
$$= -kb_M - k^2 a_M + k^2 a_{M+1}.$$

This establishes

Lemma 6.5. *The boundary condition for the left bath is given by*

$$\dot{b}_M = -kb_M - k^2 a_M + k^2 a_{M+1}, \tag{6.34}$$

where $M < 0$. Analogously, for the right boundary of the right bath we have the absorbing boundary condition

$$\dot{b}_M = -kb_M - k^2 a_M + k^2 a_{M-1}, \tag{6.35}$$

where $M > N$.

Proof. See above. $\square$

Definition 6.4. *The truncated approximations of F_L and F_R are defined by*

$$F_L^M(t) = \sum_{j=-M}^{0} a_j(t)\dot{u}_j(0) + \dot{a}_j(t)u_j(0) \tag{6.36}$$

$$F_R^M(t) = \sum_{j=N+1}^{N+1+M} a_j(t)\dot{u}_j(0) + \dot{a}_j(t)u_j(0) \tag{6.37}$$

where the a_j satisfy the following first order system

$$\dot{b}_{-M} = -kb_{-M} - k^2 a_{-M} + k^2 a_{-M+1}, \text{ (Absorbing Boundary Condition)} \tag{6.38}$$

$$\dot{a}_{-M} = b_{-M}, \tag{6.39}$$

$$\dot{a}_j = k^2(a_{j-1} - 2a_j + a_{j+1}), \text{ for } j = -1, \ldots, -M+1, \tag{6.40}$$

$$a_0(t) = \frac{2J_1(2kt)}{k^3t^2} - \frac{2J_0(2kt)}{k^2t}, \tag{6.41}$$

$$a_j = a_{N+1-j}, \text{ for } j = N+1, \ldots, (N+1)+M, \tag{6.42}$$

$$b_j = \dot{a}_j, \text{ for } j = N+1, \ldots, (N+1)+M. \tag{6.43}$$

We now prove an error estimate for the truncated approximations of the noise.

Theorem 6.6. *Fix $m \in \mathbb{N}$ and let $\mathbf{y}(t)$ and $\mathbf{y}_m(t)$ be solutions to the systems generating the noise term from theorem 6.4 and the truncated approximation of the noise definition 6.4 respectively. Then*

$$||\mathbf{y}(t) - \mathbf{y}_m(t)||_{\ell^2\times\ell^2} \leq k^2\sqrt{2}\frac{t^{2m+2}}{(2m+2)!} + O(t^{2m+3}), \tag{6.44}$$

$$||\mathbf{y}(t) - \mathbf{y}_m(t)||_{\ell^2\times\ell^2} \leq k^2\sqrt{2}\frac{t^{2m+1}}{(2m+1)!} + 2\frac{4^{2m}e^{4t}}{(2m+1)!}. \tag{6.45}$$

Proof. For ease, reindex so that the index set is now $\mathbb{N}$. Let $\mathcal{H} = \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$ and define the operators $\mathcal{L}, \mathcal{L}_m$, and $\mathbb{1}_m$ by

$$
\begin{aligned}
&\mathcal{L}\mathbf{e}_1 = \mathbf{e}_1 - \mathbf{e}_2,\\
&\mathcal{L}\mathbf{e}_j = -\mathbf{e}_{j-1} + 2\mathbf{e}_j - \mathbf{e}_{j+1}, \quad j \geq 2,\\
&\mathcal{L}_m\mathbf{e}_1 = \mathbf{e}_1 - \mathbf{e}_2,\\
&\mathcal{L}_m\mathbf{e}_j = -\mathbf{e}_{j-1} + 2\mathbf{e}_j - \mathbf{e}_{j+1}, \quad j = 2, \dots, m-1,\\
&\mathcal{L}_m\mathbf{e}_m = -\mathbf{e}_{m-1} + 2\mathbf{e}_m,\\
&\mathcal{L}_m\mathbf{e}_j = 0, \quad j > m,\\
&\mathbb{1}_m\,\mathbf{e}_j = \delta_{mj}\mathbf{e}_m,
\end{aligned}
$$

and let $\pi_m : \ell^2(\mathbb{N}) \to \ell^2(\mathbb{N})$ be the projection onto $\operatorname{span}\{\mathbf{e}_1, \dots, \mathbf{e}_m\}$. It is easy to see that $\begin{pmatrix} 0 & -\mathcal{L} \\ I & 0 \end{pmatrix}$ and $\begin{pmatrix} -k\,\mathbb{1}_m & -\mathcal{L}_m \\ \pi_m & 0 \end{pmatrix}$ are bounded operators on $\mathcal{H}$. Then $\mathbf{y}$ and $\mathbf{y}_m$ have the forms

$$
\begin{aligned}
\mathbf{y}(t) &= \int_0^t \exp\left((t-s)\begin{pmatrix} 0 & -\mathcal{L} \\ I & 0 \end{pmatrix}\right)\begin{pmatrix} 0 \\ \mathbf{e}_1 \end{pmatrix} k^2 a_0(s)ds,\\
\mathbf{y}_m(t) &= \int_0^t \exp\left((t-s)\begin{pmatrix} -k\,\mathbb{1}_m & -\mathcal{L}_m \\ \pi_m & 0 \end{pmatrix}\right)\begin{pmatrix} 0 \\ \mathbf{e}_1 \end{pmatrix} k^2 a_0(s)ds.
\end{aligned}
$$

Define $\epsilon(t) = \mathbf{y}(t) - \mathbf{y}_m(t)$. Since $\mathcal{L}, \mathcal{L}_m, \mathbb{1}_m$ and π_m are bounded operators on $\ell^2(\mathbb{N})$, and that by definition for all $j < m$ that $\mathcal{L}^j\mathbf{e}_1 = \mathcal{L}_m^j\mathbf{e}_1$, for any $\tau > 0$ we have

$$
\begin{aligned}
&\left[\exp\left(\tau\begin{pmatrix} -k\,\mathbb{1}_m & -\mathcal{L}_m \\ \pi_m & 0 \end{pmatrix}\right) - \exp\left(\tau\begin{pmatrix} 0 & -\mathcal{L} \\ I & 0 \end{pmatrix}\right)\right]\begin{pmatrix} 0 \\ \mathbf{e}_1 \end{pmatrix}\\
&= \sum_{j=0}^{\infty} \frac{\tau^j}{j!}\left[\begin{pmatrix} -k\,\mathbb{1}_m & -\mathcal{L}_m \\ \pi_m & 0 \end{pmatrix}^j - \begin{pmatrix} 0 & -\mathcal{L} \\ I & 0 \end{pmatrix}^j\right]\begin{pmatrix} 0 \\ \mathbf{e}_1 \end{pmatrix}\\
&= \sum_{j=2m}^{\infty} \frac{\tau^j}{j!}\left[\begin{pmatrix} -k\,\mathbb{1}_m & -\mathcal{L}_m \\ \pi_m & 0 \end{pmatrix}^j - \begin{pmatrix} 0 & -\mathcal{L} \\ I & 0 \end{pmatrix}^j\right]\begin{pmatrix} 0 \\ \mathbf{e}_1 \end{pmatrix}.
\end{aligned}
$$

For convenience set

$$\mathbf{s}_{m+1}(\tau) = \sum_{j=2m+1}^{\infty} \frac{\tau^j}{j!} \left[\begin{pmatrix} -k\,\mathbb{1}_m & -\mathcal{L}_m \\ \pi_m & 0 \end{pmatrix}^j - \begin{pmatrix} 0 & -\mathcal{L} \\ I & 0 \end{pmatrix}^j \right] \begin{pmatrix} 0 \\ \mathbf{e}_1 \end{pmatrix}.$$

From Taylor's theorem

$$||\mathbf{s}_{m+1}(\tau)||_{\mathcal{H}} \leq 2\frac{4^{2m+1}e^{4t}}{(2m+1)!},$$

where the 4 comes from the bound on the operator norm for the discrete Laplace operators $\mathcal{L}$ and $\mathcal{L}_m$. Then in particular, since for all $j < m$ we have $\mathcal{L}^j\mathbf{e}_1 = \mathcal{L}_m^j\mathbf{e}_1$

$$\begin{aligned}
&\sum_{j=2m}^{\infty} \frac{\tau^j}{j!} \left[\begin{pmatrix} -k\,\mathbb{1}_m & -\mathcal{L}_m \\ \pi_m & 0 \end{pmatrix}^j - \begin{pmatrix} 0 & -\mathcal{L} \\ I & 0 \end{pmatrix}^j \right] \begin{pmatrix} 0 \\ \mathbf{e}_1 \end{pmatrix} \\
&= \frac{\tau^{2m}}{(2m)!} \left[\begin{pmatrix} 0 \\ (-\mathcal{L}_m)^m\mathbf{e}_1 \end{pmatrix} - \begin{pmatrix} 0 \\ (-\mathcal{L})^m\mathbf{e}_1 \end{pmatrix} \right] + \mathbf{s}_{m+1}(\tau) \\
&= \frac{\tau^{2m}}{(2m)!} \begin{pmatrix} 0 \\ (\mathcal{L} - \mathcal{L}_m)(-\mathcal{L})^{m-1}\mathbf{e}_1 \end{pmatrix} + \mathbf{s}_{m+1}(\tau) \\
&= \frac{\tau^{2m}}{(2m)!} \begin{pmatrix} 0 \\ (\mathcal{L} - \mathcal{L}_m)\left(\mathbf{e}_m + \sum_{j=1}^{m-1} d_n\mathbf{e}_n\right) \end{pmatrix} + \mathbf{s}_{m+1}(\tau) \qquad \text{for some } d_n \in \mathbb{R} \\
&= \frac{\tau^{2m}}{(2m)!} \begin{pmatrix} 0 \\ (\mathcal{L} - \mathcal{L}_m)\mathbf{e}_m \end{pmatrix} + \mathbf{s}_{m+1}(\tau) \\
&= \frac{\tau^{2m}}{(2m)!} \begin{pmatrix} 0 \\ -e_m + \mathbf{e}_{m+1} \end{pmatrix} + \mathbf{s}_{m+1}(\tau).
\end{aligned}$$

By substituting this result into the formula for $\epsilon(t)$

$$\epsilon(t) = k^2 \int_0^t \left(\frac{(t-s)^{2m}}{(2m)!} \begin{pmatrix} 0 \\ -\mathbf{e}_m + \mathbf{e}_{m+1} \end{pmatrix} + \mathbf{s}_{m+1}(t-s) \right) a_0(s)ds.$$

Taking the norm

$$||\epsilon(t)||_{\mathcal{H}} \leq k^2 \int_0^t \left(\sqrt{2}\frac{(t-s)^{2m}}{(2m)!} + O((t-s)^{2m+1}) \right) |a_0(s)|\, ds$$

and

$$||\epsilon(t)||_{\mathcal{H}} \leq k^2 \int_0^t \left(\sqrt{2}\frac{(t-s)^{2m}}{(2m)!} + 2\frac{4^{2m+1}e^{4t}}{(2m+1)!} \right) |a_0(s)|\, ds.$$

Since a_0 is analytic on all of $\mathbb{C}$ we can Taylor expand to first order to find

$$\begin{aligned} ||\epsilon(t)||_{\mathcal{H}} &\leq k^2 \int_0^t \left(\sqrt{2}\frac{(t-s)^{2m}}{(2m)!} s \right) ds + O(t^{2m+3}) \\ &= k^2\sqrt{2}\frac{t^{2m+2}}{(2m+2)!} + O(t^{2m+3}). \end{aligned}$$

Since $a_0(t) \leq 1$ for all $t \in \mathbb{R}$, we also have the estimate

$$||\epsilon(t)||_{\mathcal{H}} \leq k^2\sqrt{2}\frac{t^{2m+1}}{(2m+1)!} + 2\frac{4^{2m}e^{4t}}{(2m+1)!}.$$

□

This error estimate can be used to give us a rough estimate for the size that the baths must be taken to be in order to guarantee sufficiently small error in some compact interval $[0, T]$. It also shows that the error goes to zero when the bath size goes to infinity.

6.2.2 Krylov Subspace Model Order Reduction

While the system of ODE's modeling the truncated approximations of the noise is particularly simple to write down, the size of the system is very large. In practice, in order for the noise term to remain acceptably accurate for the duration of the simulation, approximately $90,000$ terms are required. Yet, for the purposes of the simulation of the non-stationary GLE dynamics, the only thing that matters is the final value of F, not the exact dynamics of a ODE system which determine the truncated approximation of F. Model order reduction of single input single output (SISO) systems investigates whether smaller ODE systems driven by the same input can approximate the output function F.

A short review following [3] is presented.

Krylov Subspace Model Order Reduction: An Overview

Definition 6.5. *A continuous time-invariant single input single output (SISO) linear dynamical system is a collection of ODE's of the form*

$$C\dot{\mathbf{x}}(t) + G\,\mathbf{x}(t) = \mathbf{b}u(t), \tag{6.46}$$
$$y(t) = \mathbf{l}^T\,\mathbf{x}(t), \tag{6.47}$$

with initial condition $\mathbf{x}(0) = \mathbf{x}_0 \in \mathbb{R}^N$ *where* $t \in \mathbb{R}^+$, $\mathbf{x}(t) \in \mathbb{R}^N$, $u(t) \in \mathbb{R}$, $C, G \in \mathbb{R}^{N\times N}$, *and* $\mathbf{b}, \mathbf{l} \in \mathbb{R}^N$. *Here* t *is the time variable,* $u(t)$ *is the control or input,* $y(t)$ *is the output or observation, and* $\mathbf{x}(t)$ *is the state of the system.*

Definition 6.6. *The transfer function of a linear SISO dynamical system is the meromorphic function*

$$H(s) = \mathbf{l}^T(G + sC)^{-1}\mathbf{b}. \tag{6.48}$$

Formally, the transfer function contains all of the dynamics of the SISO system. If $h(t)$ is the inverse Laplace transform of H, then

$$y(t) = \int_0^t h(t-\tau)u(\tau)d\tau.$$

The transfer function maps Laplace transform of the input to the Laplace transform of the output, and by inverting the Laplace transform, gives us an exact representation of the output as a function of the input in time domain. Moreover if known, the transfer function eliminates the use of the state vector $\mathbf{x}(t)$ entirely. Most of the literature regarding model order reduction involves providing systematic ways to approximate the transfer function for a SISO linear dynamical system [3, 24, 20]. For frequency response and steady-state analysis, the transfer function is the primary object of study. Due to the ill posedness and conditioning of the inverse Laplace transform [10, 27], good approximations of the transfer function do not necessarily lead to good approximations in time domain. This makes transient analysis of the linear SISO system difficult. Krylov subspace techniques offer both an efficient and stable way to compute Pade approximations of the transfer function and offer methods to compute the time domain solution of a SISO dynamical system whose evolution is restricted to a relevant low dimensional (Krylov) subspace.

Definition 6.7. *The right and left nth Krylov subspace of a matrix A with starting right and left vectors $\mathbf{r}$ and $\mathbf{l}$ are*

$$K_n(A, \mathbf{r}) = span\{\mathbf{r}, A\mathbf{r}, A^2\mathbf{r}, \ldots, A^{n-1}\mathbf{r}\}, \tag{6.49}$$

$$K_n(A^T, \mathbf{l}) = span\{\mathbf{l}, A^T\mathbf{l}, \left(A^T\right)^2\mathbf{l}, \ldots, \left(A^T\right)^{n-1}\mathbf{l}\}, \tag{6.50}$$

assuming the matrix vector products $A\mathbf{r}$ and $A^T\mathbf{l}$ exist.

Typically the basis vectors as constructed in the definition are unsuitable for numerical computation. A modified version of the Lanczos process stably produces a biorthogonal set of vectors $\{\mathbf{v}_i\}_{i=1}^n \subseteq \mathbb{R}^n$ and $\{\mathbf{w}_i\}_{i=1}^n \subseteq \mathbb{R}^n$ which are bases for the left and right Krylov subspaces. We present the traditional form of Lanczos tridiagonilization, however in practice one should implement a look ahead Lanczos method as detailed in [25]. Define vectors $\{\mathbf{v}_i\}_{i=1}^n \subseteq \mathbb{R}^n$ and $\{\mathbf{w}_i\}_{i=1}^n \subseteq \mathbb{R}^n$ by the matrix recursion relations

$$AV_n = V_nT_n + \rho_{n+1}\mathbf{v}_{n+1}\mathbf{e}_n^T, \tag{6.51}$$

$$A^TW_n = W_n\widetilde{T}_n + \eta_{n+1}\,\mathbf{w}_{n+1}\,\mathbf{e}_n^T, \tag{6.52}$$

where

$$T_n = \begin{bmatrix} \alpha_1 & \beta_2 & & \\ \rho_2 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_n \\ & & \rho_n & \alpha_n \end{bmatrix}, \qquad \widetilde{T}_n = \begin{bmatrix} \alpha_1 & \gamma_2 & & \\ \eta_2 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \gamma_n \\ & & \eta_n & \alpha_n \end{bmatrix}, \tag{6.53}$$

which in turn satisfy $\widetilde{T}_n = D_n T_n D_n^{-1}$ where $D_n = W_n^T V_n = \text{diag}(\delta_1, \ldots, \delta_n)$, and where the matrices V_n and W_n are the matrices whose columns are the vectors $\{v_i\}_{i=1}^n$ and $\{w_i\}_{i=1}^n$ respectively. Throughout it is enforced that $||w_n|| = ||v_n|| = 1$ for all n. The strategy is to now to restrict the linear time invariant SISO system to these Krylov subspaces.

Definition 6.8. *Let $A = -(G + s_0 C)^{-1} C$ and $\mathbf{r} = (G + s_0 C)^{-1} \mathbf{b}$ where $s_0 \in \mathbb{R}$ is chosen so that A and r exist. Let V_n and W_n be the matrices of Lanczos vectors generated by the Lanczos process with matrix A and initial vectors $\mathbf{r}$ and $\mathbf{l}$ respectively. The nth order reduced time invariant linear SISO system is defined to be*

$$C_n \dot{\mathbf{x}}(t) + G_n \mathbf{x}(t) = \mathbf{r}_n u(t), \tag{6.54}$$
$$y_a(t) = \mathbf{l}_n^T \mathbf{x}(t), \tag{6.55}$$

where $C_n = -T_n, G_n = I - s_0 T_n, \mathbf{r}_n = \rho_1 \mathbf{e}_1, l_n = \eta_1 \delta_1 \mathbf{e}_1$.

Another Krylov Subspace Approach

The ODE presented in lemma 6.2 and theorem 6.4 on pages 97 and 99 has a simple to write down solution in operator form. In particular

$$\mathbf{a}(t) = \int_0^t \frac{\sin((t-\tau)\sqrt{\mathcal{L}})}{\sqrt{\mathcal{L}}} \mathbf{e}_1 a_0(\tau) d\tau \in \ell^2(\mathbb{N}), \tag{6.56}$$

up to reindexing. A common use of Krylov subspaces is to numerically approximate the integrand of an operator equation like above, usually representing the solution of a set of ODE's [13].

Lemma 6.7. *The Krylov subspace* $K_n(\mathcal{L}, \mathbf{e}_1) = \mathit{span}\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$.

Proof. The proof is by induction. By definition $K_1(\mathcal{L}, \mathbf{e}_1) = \text{span}\{\mathbf{e}_1\}$, establishing the base case. Assume now that $K_n(\mathcal{L}, \mathbf{e}_1) = \text{span}\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$. By definition $K_{n+1}(\mathcal{L}, \mathbf{e}_1) = \text{span}\left(K_n(\mathcal{L}, \mathbf{e}_1) \cup \{\mathcal{L}^n e_1\}\right)$. It is easy to see that $\mathcal{L}^n \mathbf{e}_1 = \sum_{j=1}^n c_j \mathbf{e}_j + \mathbf{e}_{n+1} = v + \mathbf{e}_{n+1}$ where by the inductive hypothesis $v \in K_n(\mathcal{L}, \mathbf{e}_1)$. Thus we have that $\mathbf{e}_{n+1} \in K_{n+1}(\mathcal{L}, \mathbf{e}_1)$, and thus $\text{span}\{\mathbf{e}_1, \ldots, \mathbf{e}_{n+1}\} \subseteq K_{n+1}(\mathcal{L}, \mathbf{e}_1)$. Since $\dim K_{n+1}(\mathcal{L}, \mathbf{e}_1) \leq n+1$ the result follows. □

Before we provide the proof of the error estimate, we need a lemma about repeated application of $\mathcal{L}$ in Fourier space.

Lemma 6.8. *Define the Fourier sine series transform* $U : \ell^2(\mathbb{N}) \to S = \{f \in L^2[0, 2\pi] :$ *f is odd*$\}$ *by* $U(\mathbf{e}_j) = \frac{1}{\sqrt{\pi}} \sin(jx)$. *Set* $\hat{\mathcal{L}} := U \mathcal{L} U^{-1} : S \to S$. *Then* $\hat{\mathcal{L}}^n f(x) = (2 - 2\cos(x))^n f(x)$.

Proof. We proceed by induction. First we will show that for any $f \in S$, $\hat{\mathcal{L}} f(x) = (2 - 2\cos(x)) f(x)$. It suffices to show that $\hat{\mathcal{L}} \sin(jx) = (2 - 2\cos(x)) \sin(jx)$ for all $j \in \mathbb{N}$. Calculating, fixing $j > 1$, we find

$$
\begin{aligned}
&\hat{\mathcal{L}} \sin(x) = \sqrt{\pi} U(2e_1 - \mathbf{e}_2) = 2\sin(x) - \sin(2x) = (2 - 2\cos(x))\sin(x) \\
&\hat{\mathcal{L}} \sin(jx) = \sqrt{\pi} U(-e_{j-1} + 2e_j - \mathbf{e}_{j+1}) \\
&= -\frac{e^{i(j+1)x} - e^{-i(j+1)x}}{2i} + 2\frac{e^{ijx} - e^{-ijx}}{2i} - \frac{e^{i(j-1)x} - e^{-i(j-1)x}}{2i} \\
&= \frac{e^{ijx} - e^{-ijx}}{2i}\left[2 - e^{ix} - e^{-ix}\right] \\
&= \sin(jx)(2 - 2\cos(x)).
\end{aligned}
$$

This establishes the base case. Now assume $\hat{\mathcal{L}}^n f(x) = (2 - 2\cos(x))^n f(x)$. Then since $(2 - 2\cos(x))^n f(x) \in S$ we immediately find $\hat{\mathcal{L}}^{n+1} f(x) = \hat{\mathcal{L}}(2 - 2\cos(x))^n f(x) = (2 - 2\cos(x))(2 - 2\cos(x))^n f(x) = (2 - 2\cos(x))^{n+1} f(x)$ completing the inductive step. □

Theorem 6.9. *Let $\Pi_m : \ell^2(\mathbb{N}) \to K_m(\mathcal{L}, \mathbf{e}_1) \subset \ell^2(\mathbb{N})$ be the projection map onto $K_m(\mathcal{L}, \mathbf{e}_1)$. Then*

$$\left|\left|(I - \Pi_m)\frac{\sin(\tau\sqrt{\mathcal{L}})}{\sqrt{\mathcal{L}}} e_1\right|\right|_2 \leq \frac{\tau^{2m+3}}{(2m+3)!} 2^{m+1} \sqrt{\frac{\pi}{2}\frac{(4m+4-1)!!}{(4m+4)!!}}. \tag{6.57}$$

Proof. Since $\sin(\tau x)/x$ is entire for all $\tau \in \mathbb{R}$, we have that

$$\begin{aligned} &\left|\left|(I - \Pi_m)\frac{\sin(\tau\sqrt{\mathcal{L}})}{\sqrt{\mathcal{L}}}\mathbf{e}_1\right|\right|_2 \\ &= \left|\left|\sum_{n=m+1}^{\infty} \frac{(-1)^n \tau^{2n+1}}{(2n+1)} \mathcal{L}^n \mathbf{e}_1\right|\right|_2 . \end{aligned}$$

Define the Fourier sine series transform $U : \ell^2(\mathbb{N}) \to S = \{f \in L^2[0, 2\pi] : f \text{ is odd}\}$ by $U(\mathbf{e}_j) = \frac{1}{\sqrt{\pi}} \sin(jx)$. It is well known that U is a unitary operator [59]. Set $\hat{\mathcal{L}} := U\mathcal{L}U^{-1} : S \to S$. From the previous lemma we know that $\hat{\mathcal{L}} f(x) = (2 - 2\cos(x))^n f(x)$. Thus we have that

$$\begin{aligned} &= \left|\left|\sum_{n=m+1}^{\infty} \frac{(-1)^n \tau^{2n+1}}{(2n+1)!} \mathcal{L}^n \mathbf{e}_1\right|\right|_2 \\ &= \left|\left|\sum_{n=m+1}^{\infty} \frac{(-1)^n \tau^{2n+1}}{(2n+1)!} U\mathcal{L}^n \mathbf{e}_1\right|\right|_{L^2[0,2\pi]} \\ &= \left|\left|\sum_{n=m+1}^{\infty} \frac{(-1)^n \tau^{2n+1}}{(2n+1)!} \hat{\mathcal{L}}^n U\mathbf{e}_1\right|\right|_{L^2[0,2\pi]} \\ &= \frac{1}{\sqrt{\pi}} \left|\left|\sum_{n=m+1}^{\infty} \frac{(-1)^n \tau^{2n+1}}{(2n+1)!} (2 - 2\cos x)^n \sin(x)\right|\right|_{L^2[0,2\pi]} \\ &\leq \frac{1}{\sqrt{\pi}} \left|\left|\sin(x)\right|\right|_{L^2[0,2\pi]} \left|\left|\sum_{n=m+1}^{\infty} \frac{(-1)^n \tau^{2n+1}}{(2n+1)!} (2 - 2\cos x)^n\right|\right|_{L^2[0,2\pi]} \\ &\leq \left|\left|\sum_{n=m+1}^{\infty} \frac{(-1)^n \tau^{2n+1}}{(2n+1)!} (2 - 2\cos x)^n\right|\right|_{L^2[0,2\pi]} \end{aligned}$$

$$
\begin{aligned}
&\leq \left|\left| \frac{\tau^{2m+3}}{(2m+3)!}(2-2\cos x)^{m+1} \right|\right|_{L^2[0,2\pi]} \\
&= \frac{\tau^{2m+3}}{(2m+3)!} \left|\left|(2-2\cos x)^{m+1}\right|\right|_{L^2[0,2\pi]} \\
&= \frac{\tau^{2m+3}}{(2m+3)!} 2^{m+1} \sqrt{\frac{\pi}{2}\frac{(4m+4-1)!!}{(4m+4)!!}},
\end{aligned}
$$

where !! denotes the double factorial function. The last step was computed using [26]. □

6.2.3 Spectral Evaluation of the Noise

Recall that the noise can be written as a single input single output (SISO) second order dynamical system:

$$
\ddot{\mathbf{a}} = -\mathcal{L}\mathbf{a} + \mathbf{a}_0(t)\mathbf{e}_1, \tag{6.58}
$$

$$
F(t) = \mathbf{a}(t)\cdot\dot{\mathbf{u}}(0) + \dot{\mathbf{a}}(t)\cdot\mathbf{u}(0) + a_0(t)\dot{u}_0(0) + \dot{a}_0(t)u_0(0), \tag{6.59}
$$

with $\dot{\mathbf{a}}(0) = \mathbf{a}(0) = 0$. It is easy to see that $\mathbf{a}$ has solution

$$
\mathbf{a}(t) = \int_0^t \frac{\sin\left((t-s)\sqrt{\mathcal{L}}\right)}{\sqrt{\mathcal{L}}}\mathbf{e}_1 a_0(s)ds.
$$

Differentiating we have

$$
\dot{\mathbf{a}}(t) = \int_0^t \cos\left((t-s)\sqrt{\mathcal{L}}\right)\mathbf{e}_1 a_0(s)ds.
$$

Thus both $\mathbf{a}$ and $\dot{\mathbf{a}}$ are in ℓ^2 for all $t \geq 0$ and have the form

$$
\int_0^t A_{t-s}(\sqrt{\mathcal{L}})\mathbf{e}_1 f(s)ds,
$$

where $A_\tau(z)$ is an analytic function in τ and z. The noise term however is a function involving terms of the form $\mathbf{l}^T\int_0^t A_{t-s}(\sqrt{\mathcal{L}})\mathbf{e}_1 f(s)ds$. Using Cauchy's integral formula for operator valued functions [17]

$$\begin{aligned}
&\mathbf{1}^T \int_0^t A_{t-s}(\sqrt{\mathcal{L}})\mathbf{e}_1 f(s)ds \\
&= \frac{\mathbf{1}^T}{2\pi i}\int_0^t \oint\limits_\Gamma (z-\mathcal{L})^{-1} A_{t-s}(z)\mathbf{e}_1 f(s)ds,
\end{aligned}$$

where Γ is a closed contour on the complex plain enclosing $\sigma(\mathcal{L})$, the spectrum of $\mathcal{L}$. Exchanging the order of the integrals

$$\begin{aligned}
&= \frac{\mathbf{1}^T}{2\pi i}\int_0^t \oint\limits_\Gamma (z-\mathcal{L})^{-1} A_{t-s}(z)\mathbf{e}_1 f(s)ds \\
&= \frac{\mathbf{1}^T}{2\pi i}\oint\limits_\Gamma (z-\mathcal{L})^{-1}\mathbf{e}_1 \left[\int_0^t A_{t-s}(z) f(s)ds\right] dz.
\end{aligned}$$

In a sufficiently small annulus in $\mathbb{C}$ containing Γ the function $\mathbf{e}_j(z-\mathcal{L})^{-1}\mathbf{e}_1$ is an analytic in z. Let $R(z) := \mathbf{1}^T(z-\mathcal{L})^{-1}\mathbf{e}_1$. Let $S = \{g \in L^2[0,2\pi] : g(s) = -g(-s)\}$ and let $U : \ell^2(\mathbb{N}) \to S$ be given by $U(e_j) = \frac{1}{\sqrt{\pi}}\sin(jx)$. The sine transform U is known to be unitary, and so we see that

$$\begin{aligned}
R_j(z) &= \mathbf{e}_j(z-\mathcal{L})^{-1}\mathbf{e}_1 \\
&= \langle U\mathbf{e}_j, U(z-\mathcal{L})^{-1}\mathbf{e}_1\rangle \\
&= \left\langle \sin(jx), \frac{\sin(x)}{z-k^2(2-2\cos(x))}\right\rangle \\
&= \int_0^{2\pi} \frac{1}{\pi}\frac{\sin(jx)\sin(x)}{z-2k^2+2k^2\cos(x)}dx,
\end{aligned}$$

and

$$R(z) = \sum_{j=1}^{\infty} l_j R_j(z),$$

Where $\langle\cdot,\cdot\rangle$ is the standard inner product on $\ell^2(\mathbb{N})$. Since $|z| > 4$, this integral defining

$R_j(z)$ has no convergence issues in the denominator. It turns out we can further compute $R_j(z)$ with the calculus of residues. Let $w = e^{ix}$ and performing the change of variables we find that

$$\begin{aligned} R_j(z) &= \frac{i}{4\pi} \oint_{\mathbb{S}^1} \frac{w^{j+1} - w^{j-1} - w^{-(j-1)} + w^{-(j+1)}}{k^2 w^2 + (z - 2k^2) w + k^2} dw \\ &= \frac{i}{4\pi k^2} \oint_{\mathbb{S}^1} \frac{(w^j - 1)(w^j + 1)(w + 1)(w - 1)}{w^{j+1}(w - \rho_+(z))(w - \rho_-(z))} dw \\ &= -\frac{1}{2k^2} \left[\operatorname{Res}\left(P(w), 0\right) + \operatorname{Res}\left(P(w), \rho_+(z)\right) \right], \end{aligned}$$

where $\rho_\pm(z)$ is the analytic continuation of $-(z - 2k^2) \pm \sqrt{z(z - 4k^2)}$ from the positive real line and where

$$P(w) = \frac{(w^j - 1)(w^j + 1)(w + 1)(w - 1)}{w^{j+1}(w - \rho_+(z))(w - \rho_-(z))}.$$

Note that $|\rho_-(z)| > 1$ and so the residue at the pole does not contribute to the integral. To simplify notation we set $\rho_\pm := \rho_\pm(z)$. We can now calculate the residues.

$$\begin{aligned} &\operatorname{Res}(P(w), 0) = \frac{1}{j!} \frac{d^j}{dw^j} \bigg|_{w=0} \left(\frac{w^{2j+2} - w^{2j} - w^2 + 1}{(w - \rho_+)(w - \rho_-)} \right) \\ &= \frac{1}{j!} \frac{d^j}{dw^j} \bigg|_{w=0} \left[(w^{2j+2} - w^{2j} - w^2 + 1)((w - \rho_+)(w - \rho_-))^{-1} \right] \\ &= \frac{1}{j!} \sum_{k=0}^{j} \binom{j}{k} \frac{d^k}{dw^k} \bigg|_{w=0} \left(w^{2j+2} - w^{2j} - w^2 + 1 \right) \frac{d^{j-k}}{dw^{j-k}} \bigg|_{w=0} \left((w - \rho_+)^{-1} (w - \rho_-)^{-1} \right). \end{aligned}$$

Note that $\frac{d^k}{dw^k}\Big|_{w=0} (w^{2j+2} - w^{2j} - w^2 + 1) = 0$ for all $k \neq 0, 2$. Fix $j > 1$ Then

$$\begin{aligned} \frac{d^0}{dw^0} \bigg|_{w=0} \left(w^{2j+2} - w^{2j} - w^2 + 1 \right) &= 1 \\ \frac{d^2}{dw^2} \bigg|_{w=0} \left(w^{2j+2} - w^{2j} - w^2 + 1 \right) &= -2. \end{aligned}$$

Now fix $m \in \mathbb{N}$. Then

$$\begin{aligned}
&\left.\frac{d^m}{dw^m}\right|_{w=0} \left((w-\rho_+)^{-1}(w-\rho_-)^{-1}\right) \\
&= \sum_{n=0}^{m} \binom{m}{n} \left.\frac{d^n}{dw^n}\right|_{w=0} (w-\rho_+)^{-1} \left.\frac{d^{m-n}}{dw^{m-n}}\right|_{w=0} (w-\rho_-)^{-1} \\
&= \sum_{n=0}^{m} \frac{m!}{n!(m-n)!} \frac{(-1)^n n!}{(-\rho_+)^{n+1}} \frac{(-1)^{m-n}(m-n)!}{(-\rho_-)^{m-n+1}} \\
&= \sum_{n=0}^{m} \frac{m!}{\rho_+^{n+1}\rho_-^{m-n+1}} \\
&= \frac{m!}{\rho_-^{m+1}\rho_+} \sum_{n=0}^{m} \left(\frac{\rho_-}{\rho_+}\right)^n \\
&= \frac{m!}{\rho_-^{m+1}\rho_+} \left[\frac{\left(\frac{\rho_-}{\rho_+}\right)^{m+1} - 1}{\left(\frac{\rho_-}{\rho_+}\right) - 1}\right] \\
&= m! \left[\frac{\rho_+^{-m-1} - \rho_-^{-m-1}}{\rho_- - \rho_+}\right].
\end{aligned}$$

Using these facts for $j > 1$ we have

$$\begin{aligned}
\operatorname{Res}(P(w), 0) &= \frac{1}{j!}\binom{j}{0}(1)m!\left[\frac{\rho_+^{-j-1} - \rho_-^{-j-1}}{\rho_- - \rho_+}\right] \\
&\quad + \frac{1}{j!}\binom{j}{2}(-2)(j-2)!\left[\frac{\rho_+^{-(j-2)-1} - \rho_-^{-(j-2)-1}}{\rho_- - \rho_+}\right] \\
&= \frac{\rho_+^{-j-1} - \rho_-^{-j-1}}{\rho_- - \rho_+} + \frac{1}{j!}\frac{j!}{2!(j-2)!}(-2)(j-2)!\left[\frac{\rho_+^{-j+1} - \rho_-^{-j+1}}{\rho_- - \rho_+}\right] \\
&= \frac{\rho_+^{-j-1} - \rho_-^{-j-1} - \rho_+^{-j+1} + \rho_-^{-j+1}}{\rho_- - \rho_+}.
\end{aligned}$$

For the case $j = 1$

$$\operatorname{Res}(P(w), 0) = \frac{1}{1!} \left.\frac{d}{dw}\right|_{w=0} \left(\frac{w^4 - 2w^2 + 1}{(w-\rho_+)(w-\rho_-)}\right)$$

$$= \left. \frac{(w-\rho_+)(w-\rho_-)(4w^3-4w)-(w^4-2w^2+1)(w-\rho_++w-\rho_-)}{(w-\rho_+)^2(w-\rho_-)^2} \right|_{w=0}$$
$$= \frac{\rho_+ + \rho_-}{\rho_+^2\rho_-^2}.$$

Note however that

$$\frac{\rho_+ + \rho_-}{\rho_+^2\rho_-^2} = \frac{\rho_+^{-2} - \rho_-^{-2} - 1 + 1}{\rho_- - \rho_+},$$

establishing that

$$\mathrm{Res}(P(w), 0) = \frac{\rho_+^{-j-1} - \rho_-^{-j-1} - \rho_+^{-j+1} + \rho_-^{-j+1}}{\rho_- - \rho_+},$$

for all $j \geq 1$. The residue at ρ_+ is simpler:

$$\mathrm{Res}(P(w), \rho_+) = \lim_{w \to \rho_+} \frac{w^{2j+2} - w^{2j} - w^2 + 1}{w^{j+1}(w - \rho_-)}$$
$$= \frac{\rho_+^{2j+1} - \rho_+^{2j} - \rho_+^2 + 1}{\rho^{j+1}(\rho_+ - \rho_-)}$$
$$= \frac{-\rho_+^{j+1} + \rho_+^{j-1} + \rho_+^{-j+1} - \rho_+^{-j-1}}{\rho_- - \rho_+}.$$

Combining the terms we find

$$R_j(z) = -\frac{1}{2k^2}\left[\mathrm{Res}(P(w), 0) + \mathrm{Res}(P(w), \rho_+(z))\right]$$
$$= -\frac{1}{2k^2}\left[\frac{\rho_+^{-j-1} - \rho_-^{-j-1} - \rho_+^{-j+1} + \rho_-^{-j+1}}{\rho_- - \rho_+} + \frac{-\rho_+^{j+1} + \rho_+^{j-1} + \rho_+^{-j+1} - \rho_+^{-j-1}}{\rho_- - \rho_+}\right]$$
$$= \frac{1}{2k^2}\left[\frac{-\rho_-^{-j-1} + \rho_-^{-j+1} - \rho_+^{j+1} + \rho_+^{j-1}}{\rho_+ - \rho_-}\right].$$

However it is easy to show $\rho_-^{-1} = \rho_+$:

$$\rho_-^{-1} = \frac{2k^2}{-(z-2k^2) - \sqrt{z(z-4k^2)}} = \frac{2k^2(-(z-2k^2) + 4\sqrt{z(z-4k^2)})}{z^2 - 4k^2 z + 4k^4 - z^2 + 4k^2 z} = \rho_+.$$

Hence

$$\begin{aligned} R_j(z) &= \frac{1}{2k^2}\left[\frac{-\rho_+^{j+1} + \rho_+^{j-1} - \rho_+^{j+1} + \rho_+^{j-1}}{\rho_+ - \frac{1}{\rho_+}}\right] \\ &= \frac{2}{2k^2}\left[\frac{\rho_+^j\left(-\rho_+ + \frac{1}{\rho_+}\right)}{\rho_+ - \frac{1}{\rho_+}}\right] \\ &= -\frac{1}{k^2}\rho_+^j(z). \end{aligned}$$

Thus the noise term satisfies (up to reindexing)

$$\begin{aligned} &F(t) = a_0(t)\dot{u}_0(0) + \dot{a}_0(t)u_0(0) \\ &- \frac{1}{k^2}\sum_{j=1}^{\infty}\int\limits_{\Gamma}\left[\dot{u}_j(0)\rho_+^j(z)\int_0^t \frac{\sin((t-s)z)}{z}a_0(s)ds + u_j(0)\rho_+^j(z)\int_0^t \cos((t-s)z)ds\right]dz. \end{aligned}$$

Since $|\rho_+| < 1$ on Γ, it is easy to see that $R(z)$ absolutely converges for almost every set of initial conditions $(u(0), \dot{u}(0)) \in \Omega$ (definition 2.9 on page 36). We then may apply dominated convergence so that

$$\begin{aligned} &F(t) = a_0(t)\dot{u}_0(0) + \dot{a}_0(t)u_0(0) \\ &- \frac{1}{k^2}\int\limits_{\Gamma}\left[R_u(z)\int_0^t \frac{\sin((t-s)z)}{z}a_0(s)ds + R_{\dot{u}}(z)\int_0^t \cos((t-s)z)ds\right]dz. \end{aligned}$$

This establishes

Lemma 6.10. *Let Ω be the probability space defined in definition 2.9 on page 36). Then for almost every $(u(0), \dot{u}(0)) \in \Omega$, $F(t)$ is continuous.*

Proof. Since for almost every $(u(0), \dot{u}(0)) \in \Omega$

$$F(t) = a_0(t)\dot{u}_0(0) + \dot{a}_0(t)u_0(0)$$
$$- \frac{1}{k^2} \int\limits_{\Gamma} \left[R_u(z) \int_0^t \frac{\sin((t-s)z)}{z} a_0(s)ds + R_{\dot{u}}(z) \int_0^t \cos((t-s)z)ds \right] dz$$

continuity follows from the continuity of $a_0, \dot{a}_0$ and the continuity of convolutions. $\square$

Since $R_j(z)$ explicitly known, one can compute the noise in linear time. For each z, $R(z)$ can be stably computed from the $R_j(z)$ using Horner's algorithm, and need only happen once. Moreover, since the integrals in time are convolutions of the function $a_0(t)$ and $\dot{a}_0(t)$ against sine and cosine, one can use the sum of exponentials to evaluate these convolutions linear time. Because long run times are desired, and because sine and cosine grow exponentially fast on the imaginary axis, in practice to avoid loss of precision, the contour Γ must be taken extremely close to the spectrum of $-\mathcal{L}$. When this is done, the number of random initial conditions needed to compute the resolvent R accurately grows exponentially. This expression still has great theoretical use however since it shows that the almost every sample path of the noise is continuous in time.

6.2.4 Spectral Evaluation of the Truncated Approximation of the Noise

One can try to apply the same approach to evaluate the truncated approximations of the noise spectraly. In order to calculate the truncated approximation one must solve a SISO system of the form

$$\begin{pmatrix} \dot{\mathbf{p}} \\ \dot{\mathbf{q}} \end{pmatrix} = \begin{pmatrix} -k\mathbf{e}_m \otimes \mathbf{e}_m & -\mathcal{L} \\ I & 0 \end{pmatrix} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} + a_0(t) \begin{pmatrix} \mathbf{e}_1 \\ 0 \end{pmatrix} \tag{6.60}$$
$$H(t) = \mathbf{l}_1^T \mathbf{p}(t) + \mathbf{l}_2 \mathbf{q}(t). \tag{6.61}$$

where here $\mathcal{L}$ is a discrete Laplace operator with Dirichlet boundary condition at the first index, and Neumann boundary condition at the last index. The noise $F = H(t) + g(t)$, where g is a known continuous function. Equation 6.60 has solution given by

$$\begin{pmatrix}\mathbf{p}(t)\\ \mathbf{q}(t)\end{pmatrix} = \int_0^t \exp\left[(t-s)\begin{pmatrix}-k\mathbf{e}_m\otimes\mathbf{e}_m & -\mathcal{L}\\ I & 0\end{pmatrix}\right]\begin{pmatrix}\mathbf{e}_1\\ 0\end{pmatrix} a_0(s)ds. \tag{6.62}$$

Using the Cauchy integral formula we then may write H as

$$H(t) = \frac{1}{2\pi i}\int\limits_{\Gamma}\begin{pmatrix}\mathbf{l}_1\\ \mathbf{l}_2\end{pmatrix}^T\left(z-\begin{pmatrix}-k\mathbf{e}_m\otimes\mathbf{e}_m & -\mathcal{L}\\ I & 0\end{pmatrix}\right)^{-1}\begin{pmatrix}\mathbf{e}_1\\ 0\end{pmatrix}\int_0^t e^{(t-s)z}a_0(s)ds$$

$$\frac{1}{2\pi i}\int\limits_{\Gamma}\begin{pmatrix}\mathbf{l}_1\\ \mathbf{l}_2\end{pmatrix}^T\begin{pmatrix}z+k\mathbf{e}_m\otimes\mathbf{e}_m & \mathcal{L}\\ I & z\end{pmatrix}^{-1}\begin{pmatrix}\mathbf{e}_1\\ 0\end{pmatrix}\int_0^t e^{(t-s)z}a_0(s)ds.$$

where Γ is a contour containing the spectrum of $\begin{pmatrix}-k\mathbf{e}_m\otimes\mathbf{e}_m & -\mathcal{L}\\ I & 0\end{pmatrix}$. Performing the Schur complement on the first piece we get

$$H(t) = \frac{1}{2\pi i}\int\limits_{\Gamma}\begin{pmatrix}\mathbf{l}_1\\ \mathbf{l}_2\end{pmatrix}^T\begin{pmatrix}(z+k\mathbf{e}_m\otimes\mathbf{e}_m+\frac{1}{z}\mathcal{L})^{-1}\mathbf{e}_1\\ \frac{1}{z}(z+k\mathbf{e}_m\otimes\mathbf{e}_m+\frac{1}{z}\mathcal{L})^{-1}\mathbf{e}_1\end{pmatrix}\int_0^t e^{(t-s)z}a_0(s)ds.$$

Note that for each z, $(z+k\mathbf{e}_m\otimes\mathbf{e}_m+\frac{1}{z}\mathcal{L})$ is a tridiagonal matrix, and only needs to be computed once for each z. This allows for efficient computation of the resolvent. Moreover, the convolution in time can again be efficiently computed by the fast convolution for the sum of exponentials.

Remark. *Unfortunately, computing the noise and the truncated approximation of the noise spectrally did not work in practice. This is due to where contour is placed. However, this method is likely to work for long time calculations of large, possibly infinite, SISO systems whose infitessimal generator of the semigroup generating the flow (when formulated as a first order system) has spectrum well seperated from the imaginary axis.*

6.2.5 Experiments and Results

We simulate equations beginning at equation (6.15) on page 95 using the truncated approximations of the noise terms defined 6.4. The random initial conditions of the bath degrees of freedom are precomputed according to the measure defined in chapter 2. In particular, the positions are mean zero Gaussian random variables with covariance given by theorem 2.10. We use 90,000 terms to evaluate the truncated approximation of the noise. A sum of exponentials approximation of the memory kernel θ is precomputed by the matrix pencil method as follows. A discrete sum of exponentials approximation is generated by samples of θ on a coarse grid of discretization size 0.2, which is then used to produce a continuous sum of exponentials approximation.

A third order Runge-Kutta integrator is used for the non-stationary GLE's. At each time step, the convolution is evaluated via the fast convolution for sum of exponentials presented in equation 6.3, where the integral is approximated via the trapezoidal rule. The ODE's governing the truncated approximations of the noise are integrated on the fly with third order Runge-Kutta. Samples of the displacement and velocities are taken at regular intervals after reaching a predefined equilibriation time. After the simulation has concluded, time averages of the observables of interest presented in chapter 1 are computed. The method is second order accurate in time.

Systems of size $N = 2^n, n = 4, \ldots, 10$ were simulated. Each system size was simulated with bath temperatures $T_L = 0.002, T_R = 0.008$, $T_L = 0.02, T_R = 0.08$, $T_L = 0.2, T_R = 0.8$, $T_L = 0.5, T_R = 0.5$, and $T_L = 2, T_R = 8$. This resulted in a total of 35 simulations. Each simulation had a final time of $10,000$, an equilibriation time of 5000 and a time step of $\Delta t = 0.001$. After the equilibriation time is reached, samples of the positions and velocities of each particle were taken every one hundred time steps. Random initial conditions were used: the initial velocities of the particles of the resolved system were normally distributed $\mathcal{N}(0, (T_L + T_R)/2)$ and the initial displacements were uniformly distributed in $(-a/4, a/4)$.

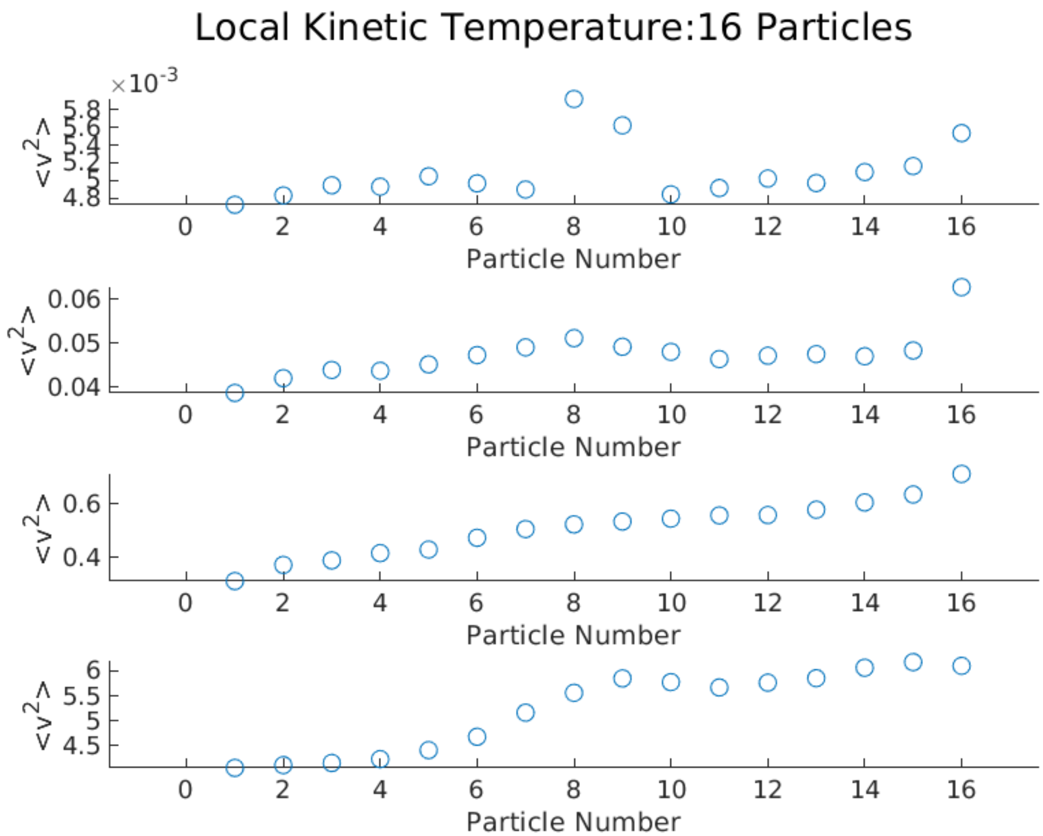
Equilibriation tests: The simulations where $T_L = T_R = 0.5$ are equilibriation tests and verify no anomalous behavior is present when the baths are at the same temperature. Figure 6.1 beginning on page 183 shows the local kinetic temperature profile for different system sizes. The temperature profile is visibly flat with no anomalous behavior present in the bulk or at the interfaces.

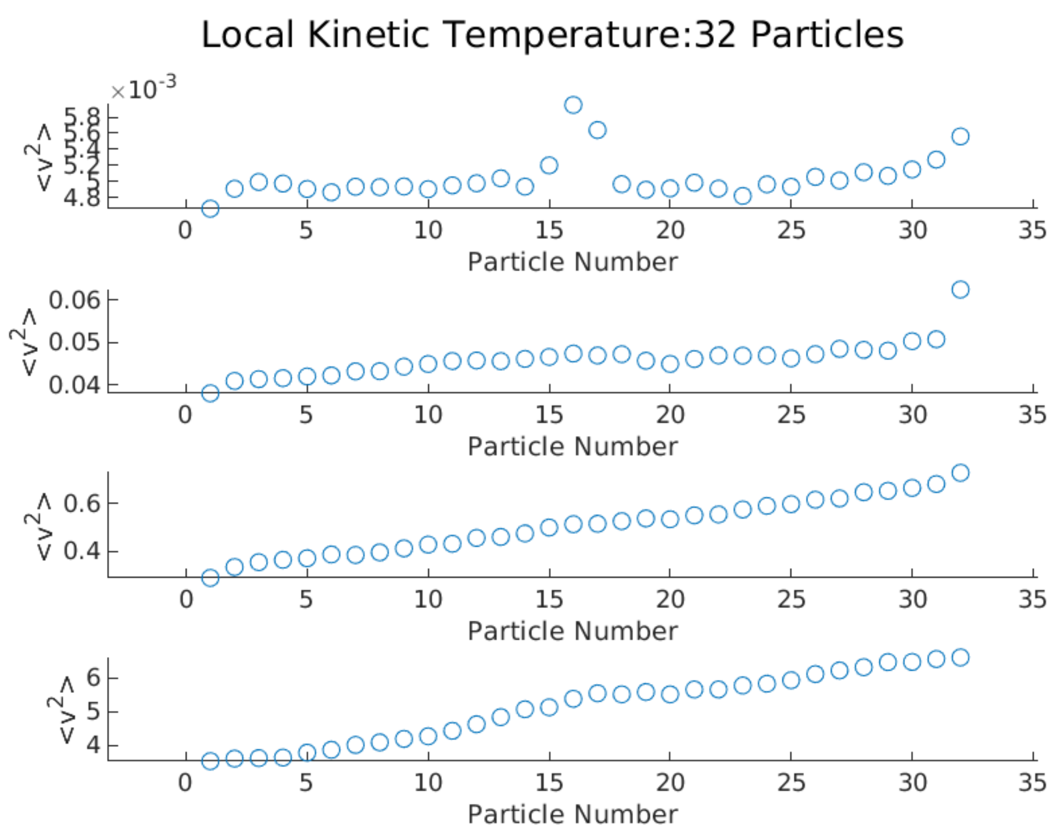
Non-Equilibrium Experiments: Figure 6.2 displays the local kinetic temperatures of the systems at temperatures, $T_L = 0.002, T_R = 0.008$, $T_L = 0.02, T_R = 0.08$, $T_L = 0.2, T_R = 0.8$, and $T_L = 2, T_R = 8$. When the bath temperatures are $T_L = 0.002, T_R = 0.008$, anomalous behavior is present at all system scales. The temperature of the boundary particles is discontinuous from the the bath temperatures. Another discontinuity in the temperature profile between the boundary particles and their neighbors in the resolved system is also present. The bulk of the resolved system is then approximately constant in temperature. The temperature of the system with 1024 particles seems to experience a small gradient in the bulk, but because of the small temperature and temperature difference, this may simply be an artifact.

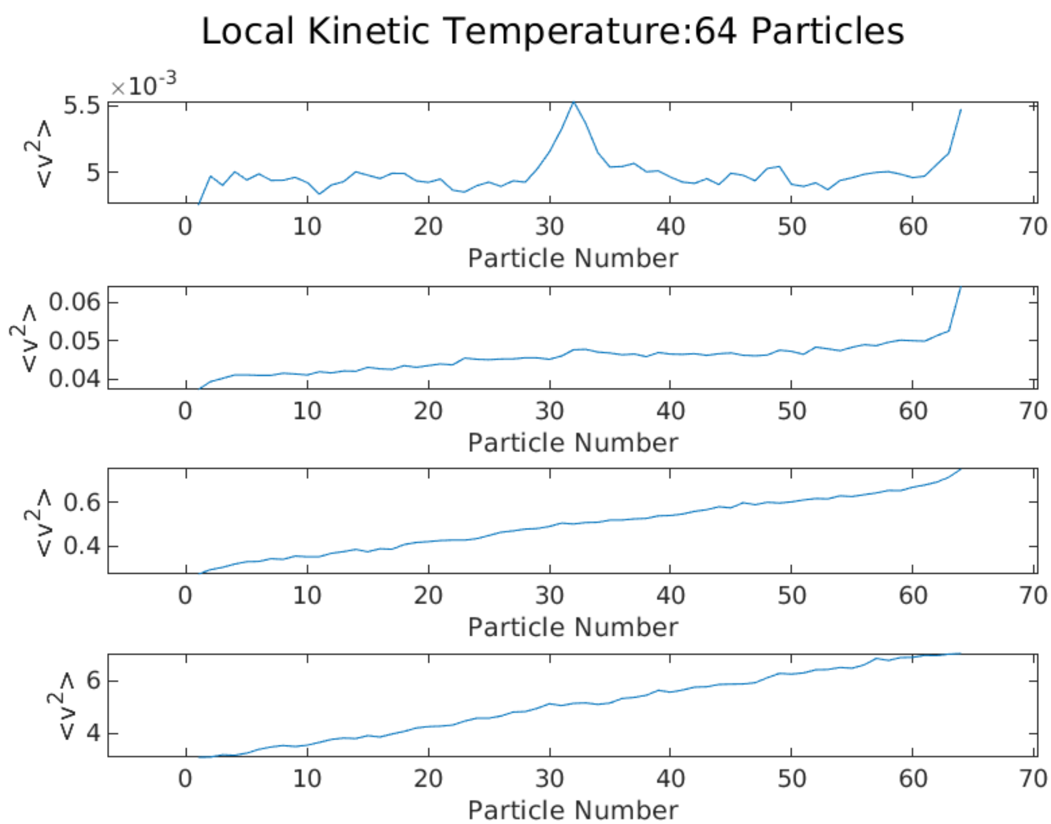
When the temperatures of the baths are selected to be $T_L = 0.02$ and $T_R = 0.08$ the temperature profile has strong non-linear or discontinuous behavior at the interfaces for systems of size 256 or less. When the system size is increased to 512 or 1024 particles, this behavior is damped, but there is still clear non-linear and anomalous behavior happening even at these scales. Moreover, the local temperature of the boundary particles never fully reaches the selected bath temperature for any of the system sizes, and the boundary particles fail to fully reach the temperature of the baths for all system sizes at this temperature.

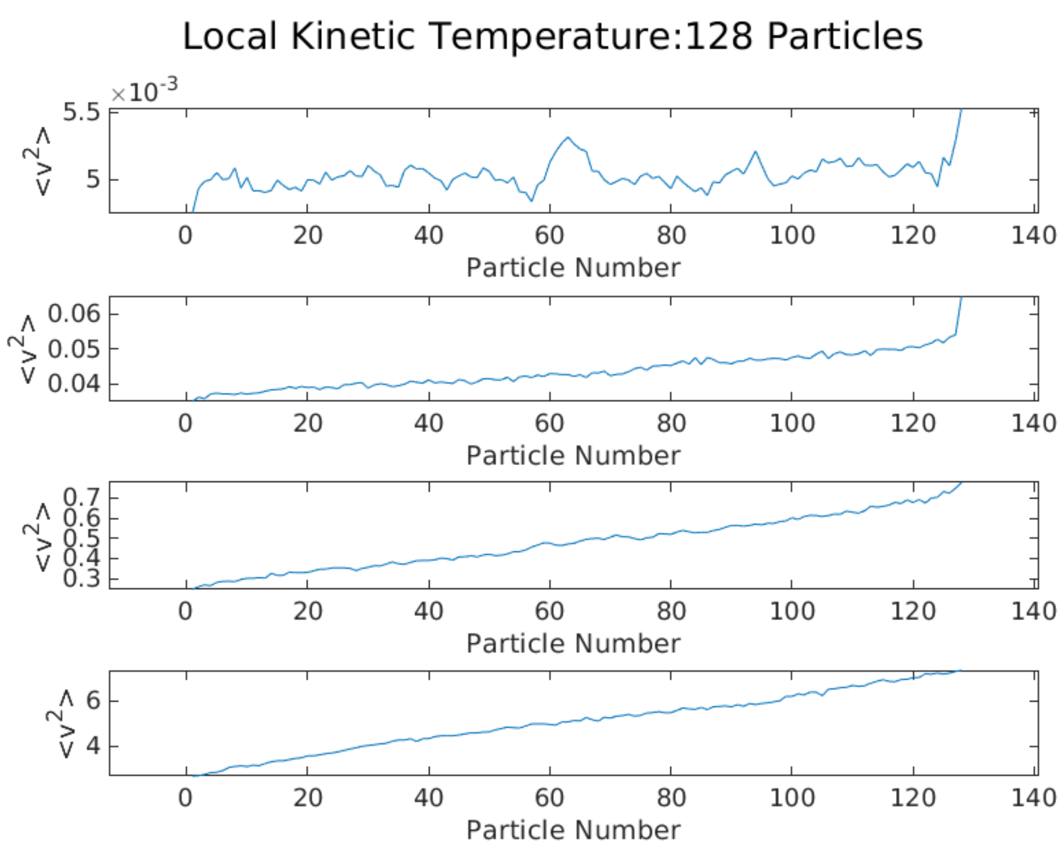
Increasing the temperature to $T_L = 0.2$ and $T_R = 0.8$ reduces the anomalous behavior. At this setting, clear but mild non-linearities are visible for systems of size up to 32. However, when the system size is increased past this point the temperature profile becomes linear. The local temperature of the boundary particles fails reach the selected bath temperatures until the system size is 256.

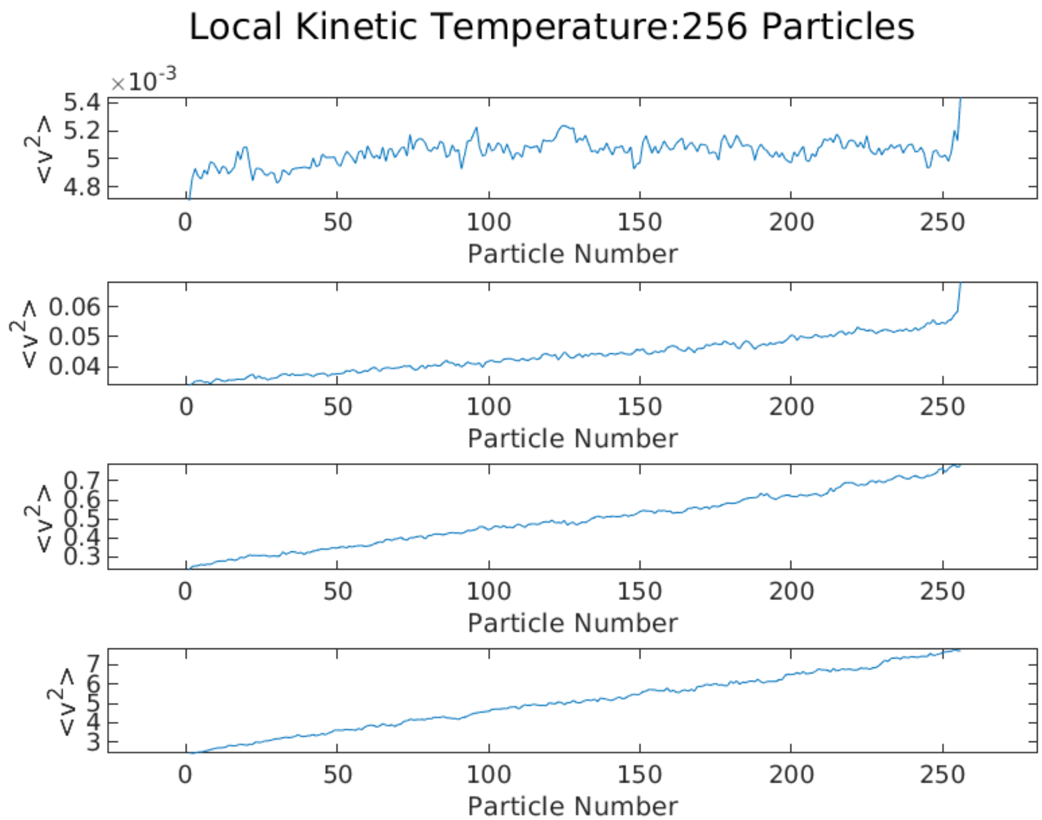
Further increasing the temperatures to $T_L = 2$ and $T_R = 8$ continues to reduce the anomalous behavior of the local kinetic temperature. However for systems of size 16 and 32 a clear non-linear behavior is still present near the center of the resolved system. For these systems, the boundary particles fail to reach the selected bath temperatures. The temperature profile is then relatively flat by the boundary particles with a sudden gradient present in the center of the resolved system. For larger systems this behavior becomes damped. The temperature discontinuity between the bath and boundary particles and the non-linearity of the temperature profile is present until the system size is chosen to be 128 particles.


Local Kinetic Temperature:16 Particles
×10^-3
<v^2>
Particle Number


Local Kinetic Temperature:32 Particles
×10^-3
<v^2>
Particle Number


Local Kinetic Temperature:64 Particles
<v^2>
Particle Number


Local Kinetic Temperature:128 Particles
<v^2>
Particle Number


Local Kinetic Temperature:256 Particles
×10^-3
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5.2
5
4.8
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50
100
150
200
250
Particle Number
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0.05
0.04
0.7
0.6
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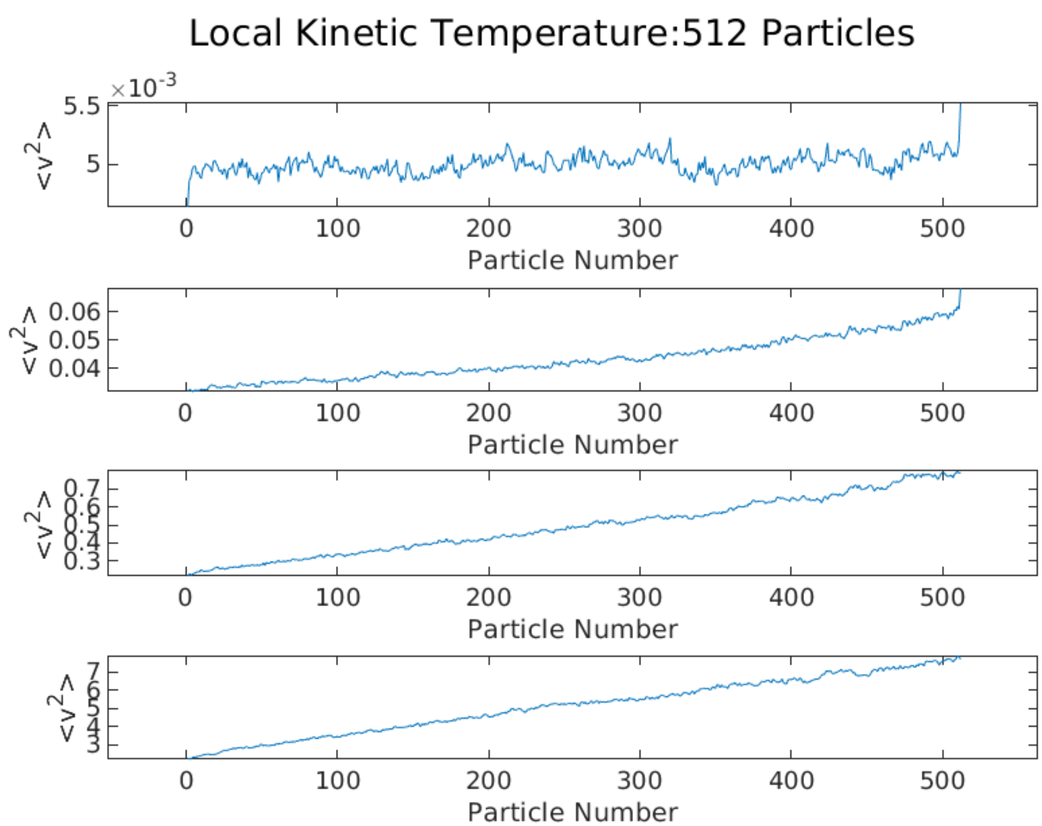
0.4
0.3
7
6
5
4
3


Local Kinetic Temperature:512 Particles
×10^-3
5.5
5
<v^2>
0
100
200
300
400
500
Particle Number
0.06
0.05
0.04
0.7
0.6
0.5
0.4
0.3
7
6
5
4
3

T_L - T_R	α	α°	$\alpha^\circ - \alpha$
0.002 - 0.008	2.0021	1.20024	3×10^{-4}
0.02 - 0.08	1.7065	1.7079	1.4×10^{-3}
0.2 - 0.8	1.3579	1.3565	-1.4×10^{-3}
2 - 8	1.2055	1.1938	-1.17×10^{-2}

Table 6.1: Conductivity Scaling Coefficients - Non-Stationary GLE

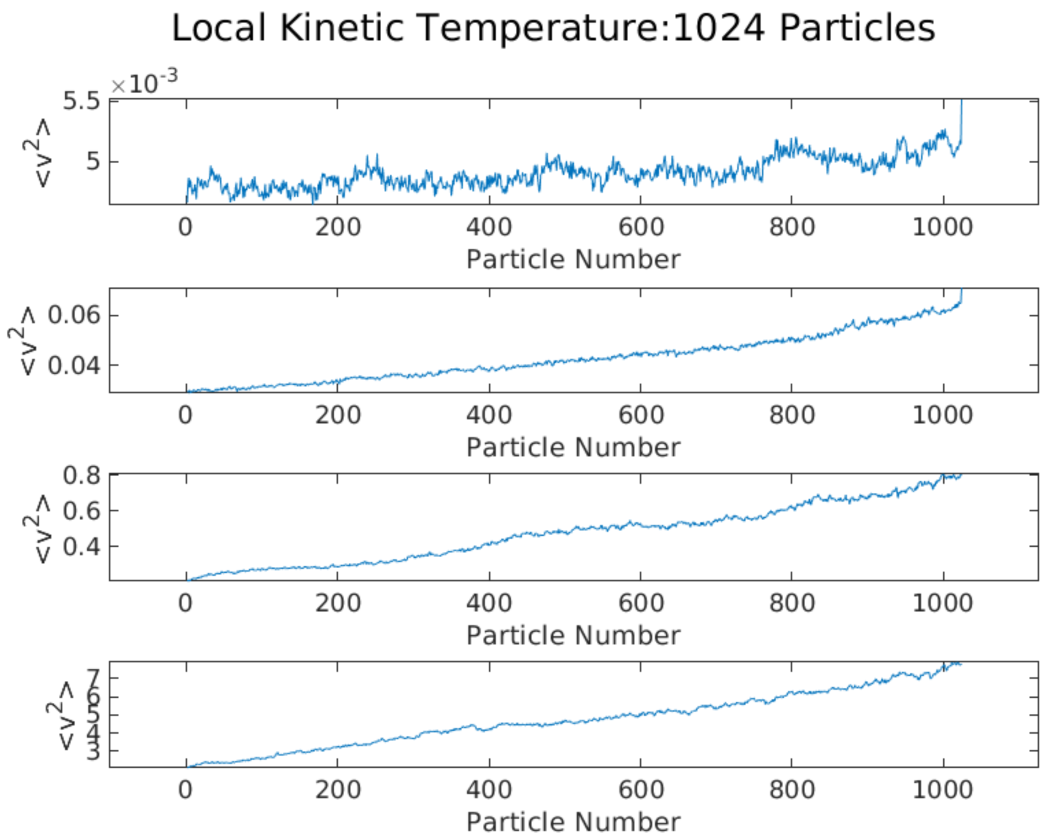


Figure 6.2: Local Kinetic Temperature - Non-Stationary GLE: Anomalous behavior visible for smaller lower temperature difference systems.

Figures 6.3 and 6.4 beginning on page 184 respectively plot $\log \kappa$ and $\log \kappa^o$ vs $\log N$. The linearity present in these plots indicate that κ and κ^o scales as N^α and N^{α^o} respectively. Table 6.1 on page 125 displays the values of α and α^o, and their differences. The largest difference between α and α^o is of the order 10^{-2}, indicating the limit of small oscillations is valid for this system. As the temperature difference and average temperature are increased the conductivity scaling coefficients decrease. However positive values of α and α^o show the divergence of conductivity indicating the failure of Fourier's law.

6.3 Stationary GLE Solutions

Corollary 4.13 on page 75 is a surprising and important result. The failure of the fluctuation dissipation theorem comes from the fact that the noise term is not stationary. Stationarity gives an analytic time domain representation of the correlation function of noise and allows for the quick and efficient sampling of the noise. Most interestingly however, if one demands that the noise is stationary, and thus that the fluctuation dissipation theorem holds, one can easily investigate the roll of memory on evolution and non-equilibrium stationary state observables of the system. The most extreme of these truncations is when memory is removed entirely by replacing the memory kernel with a Dirac delta, resulting in a Langevin equation.

Definition 6.9. *Given a memory kernel $\kappa : \mathbb{R} \to \mathbb{R}$, the stationary GLE's are defined to be the stochastic integrodifferential equations of the form*

$$\ddot{u}_1 = \phi'(u_2 - u_1 + a) - k^2 \int_0^t \kappa(t-s)\dot{u}_1(s)ds + k^2 F_L(t), \tag{6.63}$$

$$\ddot{u}_j = \phi'(u_{j+1} - u_j + a) - \phi'(u_j - u_{j-1} + a), \quad j = 2, \dots, N-1, \tag{6.64}$$

$$\ddot{u}_N = -\phi'(u_{N-1} - u_N + a) - k^2 \int_0^t \kappa(t-s)\dot{u}_N(s)ds + k^2 F_R(t). \tag{6.65}$$

where F_L, F_R are stationary Gaussian processes with correlations functions satisfying the fluctuation dissipation theorem:

$$\langle F_L(0)F_L(t)\rangle = k_B T_L \kappa(t), \tag{6.66}$$

$$\langle F_R(0)F_R(t)\rangle = k_B T_R \kappa(t). \tag{6.67}$$

6.3.1 Truncation and Scaling the Memory Kernel

In order to investigate the roll of memory on the observables of the system, one must determine a systematic way of truncating and scaling the memory kernel in a way which attempts to meet the following criterion.

- The truncated memory kernel θ_T is entirely, or almost entirely unchanged on some $[0, T]$, save for a constant rescaling, and is either zero or rapidly vanishes to zero on (T, ∞).

- That $\int_0^\infty \theta_T(t)dt = \int_0^\infty \theta(t)dt$. This is a normalization condition enforcing the Kubo formula for the thermal transport coefficient [4].

- That θ_T is a positive definite function for all truncation times T. Without this condition, the θ_T cannot be the correlation function of a stationary Gaussian process.

As a first guess one may set $\theta_T(t) = c\chi_{[0,T]}(t)\theta(t)$, where $\chi_{[0,T]}$ is the characteristic function of $[0, T]$ and $c \in \mathbb{R}$ is an appropriately chosen normalization. Doing so, or similarly with a smooth bump function, results in a truncated memory kernel which is not positive definite. Instead we use a Gaussian.

Definition 6.10. *Fix $\epsilon, T_c > 0, 0 < r < 1$ and let $T = T_c\sqrt{\frac{\log \epsilon}{\log r}}$. A truncated version of the memory kernel θ, denoted θ_T satisfies*

$$\theta_T(t) = cr^{\left(\frac{t}{T_c}\right)^2}\theta(t), \tag{6.68}$$

$$c^{-1} = k\int_0^\infty r^{\left(\frac{t}{T_c}\right)^2}\theta(t)dt. \tag{6.69}$$

It will turn out that this definition for the truncated memory kernel will satisfy the previously outlined properties. But before proving that it is necessary to show that the normalization coefficient $c > 0$.

Lemma 6.11. *Let θ_T be a truncated version of the memory kernel. Then the normalization coefficient $c > 0$.*

Proof. First note that the integral is well defined and finite since both $r^{\left(\frac{t}{T_c}\right)^2}, \theta(t) \in L^2(\mathbb{R})$. To show $c > 0$ it suffices to show that $\int\limits_0^\infty r^{\left(\frac{t}{T_c}\right)^2}\theta(t)dt > 0$. Since θ is even, the integrand is even and we have that

$$\int\limits_0^\infty r^{\left(\frac{t}{T_c}\right)^2}\theta(t)dt = \frac{1}{2}\int\limits_{-\infty}^\infty r^{\left(\frac{t}{T_c}\right)^2}\theta(t)dt = \frac{1}{2}\left\langle r^{\left(\frac{t}{T_c}\right)^2}, \theta(t)\right\rangle,$$

where $\langle\cdot,\cdot\rangle$ is the standard $L^2(\mathbb{R})$ inner product. Thus showing $a > 0$ further reduces to showing $\left\langle r^{\left(\frac{t}{T_c}\right)^2}, \theta(t)\right\rangle > 0$. From the unitarity of the Fourier transform

$$\left\langle r^{\left(\frac{t}{T_c}\right)^2}, \theta(t)\right\rangle = \left\langle \widehat{r^{\left(\frac{t}{T_c}\right)^2}}(\xi), \hat{\theta}(\xi)\right\rangle,$$

Where we use the notation $\widehat{f}$ to denote the Fourier transform of a function $f \in L^2(\mathbb{R})$ [59]. Since $r^{\left(\frac{t}{T_c}\right)^2} = e^{-\left(\frac{\log r^{-1}}{T_c^2}\right)t^2}$ we find that

$$\widehat{r^{\left(\frac{t}{T_c}\right)^2}}(\xi) = \frac{T_c}{\sqrt{2\log r^{-1}}}e^{-\left(\frac{T_c^2}{4\log r^{-1}}\right)\xi^2} > 0.$$

We now will show that $\hat{\theta}(\xi) \geq 0$ for all $\xi \in \mathbb{R}$. Recall that $\theta(t) = \dfrac{J_1(2kt)}{kt}$. Since the Fourier transform sends products to convolutions we have $\hat{\theta}(\xi) = \frac{1}{k}\left[\widehat{\frac{1}{t}}(\xi) * \widehat{J_1(2kt)}(\xi)\right]$. These Fourier transforms have well known forms [26]:

$$\widehat{\frac{1}{t}}(\xi) = -i\sqrt{\frac{\pi}{2}}\mathrm{sgn}(\xi),$$
$$\widehat{J_1(2kt)}(\xi) = \frac{1}{2k}\sqrt{\frac{2}{\pi}}\frac{-i\frac{\xi}{2k}\mathrm{rect}\left(\frac{\xi}{2k}\right)}{\sqrt{1-\frac{\xi^2}{4k^2}}},$$

where $\mathrm{sgn}(\xi) = \frac{\xi}{|\xi|}$ and $\mathrm{rect}(\xi) = \chi_{[-\frac{1}{2},\frac{1}{2}]}(\xi)$ is the characteristic function on $[-\frac{1}{2},\frac{1}{2}]$. One can then show that

$$\hat{\theta}(\eta) = \frac{-1}{2k}\mathrm{sgn}(\xi) * \frac{\xi\mathrm{rect}\left(\frac{\xi}{4k}\right)}{\sqrt{4k^2-\xi^2}}(\eta).$$

If $\Xi(\eta) := \mathrm{sgn}(\xi) * \frac{\xi\mathrm{rect}\left(\frac{\xi}{4k}\right)}{\sqrt{4k^2-\xi^2}}(\eta) \leq 0$ for all $\xi \in \mathbb{R}$ and $\Xi(\eta)$ is supported on a set of positive measure then the lemma is proved. Note that $\Xi(\eta)$ is even since it is the convolution of odd functions. Explicitly, since $k > 1$,

$$\Xi(\eta) = \int_{-4k}^{4k} \frac{\xi\mathrm{sgn}(\eta-\xi)}{\sqrt{4k^2-\xi^2}}d\xi.$$

If $\eta \geq 4k$, then

$$\Xi(\eta) = \int_{-4k}^{4k} \frac{\xi}{\sqrt{4k^2-\xi^2}}d\xi = 0,$$

since the integrand is odd. Fix $\eta \in [0, 4k]$. Then

$$\begin{aligned}\Xi(\eta) &= \int\limits_{-4k}^{-\eta} \frac{\xi}{\sqrt{4k^2-\xi^2}}d\xi + \int\limits_{-\eta}^{\eta} \frac{\xi}{\sqrt{4k^2-\xi^2}}d\xi + \int\limits_{\eta}^{4k} \frac{\xi(-1)}{\sqrt{4k^2-\xi^2}}d\xi \\ &= -2\int_{\eta}^{4k} \frac{\xi}{\sqrt{4k^2-\xi^2}}d\xi < 0.\end{aligned}$$

Evenness of Ξ shows that $\Xi(\eta) \leq 0$ for all $\eta \in \mathbb{R}$ and that the support of Ξ is $[-4k, 4k]$ completing the proof. □

Lemma 6.12. *Fix $\epsilon, T_c > 0, 0 < r < 1$ and let $T = T_c\sqrt{\frac{\log\epsilon}{\log r}}$. The truncated version θ_T be a truncated version of the memory kernel θ. Then θ_T satisfies the following:*

1. *$\theta_T(t) = O\left(r^{\left(\frac{t}{T_c}\right)^2}\right)$ as $t \to \infty$ and $||\theta_T||$.*

2. *$\int_0^\infty \theta_T(t)dt = \int_0^\infty \theta(t)dt$.*

3. θ_T is a positive definite function.

Proof. We will prove the parts of the lemma in order. Note that item *1* is immediate from the definition of the truncated version of the memory kernel θ. The second part of the lemma also follows from the definition, since $\int_0^\infty \theta(t)dt = \frac{1}{k}$. It simply remains to show that Θ_T is a positive definite function. By Bochner's theorem [8] it suffices to show that there exists a non-negative function $\phi : \mathbb{R} \to \mathbb{R}$ such $\theta(t) = \hat{\phi}(t)$, where, again, $\hat{f}$ denotes the Fourier transform of $f \in L^2(\mathbb{R})$. If such a ϕ existed, then parity symmetry of the Fourier transform would demand that $\phi(\xi) = \widehat{\theta_T}(-\xi)$. Since $\theta_T \in L^2(\mathbb{R})$ this ϕ exists and one need only verify that $\phi(\xi) = \widehat{\theta_T}(-\xi) \geq 0$ for all $\xi \in \mathbb{R}$ and ϕ is supported on a set of positive measure. Note that

$$\widehat{\theta_T}(-\eta) = \widehat{cr^{\left(\frac{t}{T_c}\right)^2}}(\xi) * \hat{\theta}(\xi)(-\eta).$$

From the proof of the lemma 6.11 we have that

$$\begin{aligned} \hat{\theta}(\xi) &= -\frac{1}{2k}\Xi(\xi) \geq 0, \\ \widehat{r^{\left(\frac{t}{T_c}\right)^2}}(\xi) &= \frac{T_c}{\sqrt{2\log r^{-1}}} e^{-\left(\frac{T_c^2}{4\log r^{-1}}\right)\xi^2} > 0, \end{aligned}$$

for all $\xi \in \mathbb{R}$. Since the convolution of non-negative functions is non-negative, both functions are supported on sets of positive measure, and from lemma 6.11, $c > 0$, we have that $\phi(\xi) \geq 0$ completing the proof. □

6.3.2 Sampling the Noise

In [14] Dietrich and Newman outline a general method to efficiently sample stationary Gaussian processes exactly on a uniformly spaced mesh. The method is summarized as follows. Suppose that F is a stationary Gaussian process with covariance function $R(x) = \langle F(x)F(0)\rangle$, where $\langle\cdot\rangle$ denotes expected value with respect to the probability space underlying the stochastic process F. Let $\{x_j\}_{j=0}^m$ be a uniformly spaced mesh of sample points, and $r_j = R(|x_j - x_0|)$, $j = 0, \ldots, m$ be $m+1$ equally spaced samples of R. Let r be the $(m+1) \times (m+1)$ symmetric Toeplitz matrix whose first row is $r_0, \ldots, r_m$. Choose $M \geq m$ and from these samples build the symmetric Teoplitz matrix $S \in M_{2M}$ whose first row $\mathbf{s}^T = (s_0, \ldots s_{2M})$ is defined by

$$\begin{aligned} s_k &= r_k & k &= 0, \ldots m, \\ s_{2M-k} &= r_k, & k &= 1, \ldots m-1, \end{aligned}$$

where if $M > 0$, the choices of the unspecified entries is entirely judiciously or randomly chosen. By construction S is circulant and is thus diagonalized by the discrete Fourier transform:

$$S = \frac{1}{2M} F \Lambda F^*,$$

where Λ is diagonal, $F_{pq} = e^{2\pi i pq/2M}$ is the matrix representation of the discrete Fourier operator, and * denotes conjugate transpose. Suppose now that S is non-negative definite and set $\tilde{\mathbf{s}} = F\,\mathbf{s}$. Let $\mathbf{e} = \mathbf{e}_1 + i\mathbf{e}_2$ where $\mathbf{e}_1, \mathbf{e}_2 \in \mathbb{R}^{2M}$ are mean zero normally distributed random vectors with covariance $\langle \mathbf{e}_j \mathbf{e}_k^T \rangle = \delta_{jk} I$. Here δ_{jk}, $j, k = 1, 2$ is the Knonecker delta function, and I is the $2M \times 2M$ identity matrix. Set $\mathbf{f}_S = F\sqrt{\frac{\Lambda}{2M}}\mathbf{e}$. By construction the real and imaginary parts of $\mathbf{f}_S$ are independent mean zero normal random vectors with covariance matrix S. If we define $\mathbf{f}$ to be the first $m+1$ entries of $\mathbf{f}_S$ then we recover two independent mean zero normal random vectors whose covariance matrix is r by taking the real and imaginary parts of $\mathbf{f}$ since, by construction, any $(m+1) \times (m+1)$ block submatrix on the diagonal of S is a copy of r. In practice the algorithm is implemented as follows:

1. Form the vector $\mathbf{s}$ from the samples of R on $\{x_j\}_{j=0}^m$.

2. Compute the fast Fourier transform of $\mathbf{s}$ and store as $\tilde{\mathbf{s}}$.

3. Sample $\mathbf{e}_1, \mathbf{e}_2$, two i.i.d $N(0, I)$ vectors of length $2M$ and form $\mathbf{e} = \mathbf{e}_1 + i\mathbf{e}_2$.

4. Compute $\tilde{\mathbf{f}} \in \mathbb{C}^{2M}$ where $\tilde{\mathbf{f}}_j = \mathbf{e}_j \sqrt{\frac{\tilde{\mathbf{s}}_j}{2M}}$.

5. Compute the fast Fourier transform of $\tilde{\mathbf{f}}$ and store as $\mathbf{f}_S$.

6. The first $(m+1)$ entries of $\Re(\mathbf{f}_S)$ and $\Im(\mathbf{f}_S)$ are two independent samples of F on $\{x_j\}_{j=0}^{m}$.

The most expensive numerical operation for this method is the computation of the FFT's, and as a result the algorithm requires only $O(M \log M)$ total operations. Further it only requires $O(M)$ memory. The condition that the matrix S is non-negative definite is not automatic in general. In [14], the bulk of the paper is investigating conditions under which the minimal embedding of $m = M$ is sufficient for S to be non-negative definite. It turns out however that sufficiently large samples of both θ and θ_T admit minimal embeddings.

Theorem 6.13. *For every $l > \frac{1}{4k}$ (resp. $l > 0$) there exists a positive integer m depending on l such that the vector with entries $\theta\left(\frac{j}{l}\right)$ (resp. $\theta_T\left(\frac{j}{l}\right)$) $j = 0, \dots m$ admits a non-negative definite embedding,*

Proof. The proof simply check that one can apply corollary 2 of [14] to θ and θ_T. Note that both $\theta, \theta_T \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, and are smooth. Further from the proof of 6.12 on page 129 and properties of convolutions [59] we know that $\widehat{\theta_T}$ and $\hat{\theta}$ are both continuous, where again $\hat{f}$ denotes the Fourier transform of $f \in L^2(\mathbb{R})$. With the above conditions and evenness of θ and θ_T, the Fourier sampling theorem presented in [8] establishes the following equalities:

$$l \sum_{j=-\infty}^{\infty} \hat{\theta}\left(\frac{\omega}{l} - jl\right) = \theta(0) + 2\sum_{j=1}^{\infty} \theta\left(\frac{j}{l}\right) \cos(2\pi j\omega) := \widetilde{s}_l(\omega),$$
$$l \sum_{j=-\infty}^{\infty} \widehat{\theta}_T\left(\frac{\omega}{l} - jl\right) = \theta(0) + 2\sum_{j=1}^{\infty} \theta_T\left(\frac{j}{l}\right) \cos(2\pi j\omega) := \widetilde{s}_l^T(\omega).$$

Note that by construction $\tilde{s}_l$ and $\widetilde{s_l^T}$ are periodic of period 1. To apply corollary 2 of [14] and prove the theorem it suffices to check that for any $\omega \in [0, 1]$, that $\widetilde{s_l^T}(\omega), \widetilde{s_l}(\omega) > 0$. We begin with the checking that $\widetilde{s_l}(\omega) > 0$. Assume $l > \frac{1}{4k}$. Then for any $\omega \in [0, 1]$ we have $\frac{\omega}{l} < 4k$, and thus, since $k > 1$,

$$\hat{\theta}\left(\frac{\omega}{l}\right) = \frac{1}{k} \int_{\frac{\omega}{l}}^{4k} \frac{\eta}{\sqrt{4k^2 - \eta^2}} d\eta > 0,$$

since the integrand is strictly positive on a positive measure set. Since from the proof of lemma 6.12 we known that $\hat{\theta}(\xi) \geq 0$ for all $\xi \in \mathbb{R}$, it immediately follows that $\widetilde{s_l}(\omega) > 0$. Now instead suppose that merely $l > 0$. Then from properties of the convolution and the proof of 6.12 we know that $\widehat{\theta_T}(\xi) > 0$ since $\widehat{\theta_T}$ is the convolution of a strictly positive function with a non-negative function supported on a set of positive measure, and thus $\widetilde{s_l^T}(\omega) > 0$. $\square$

Theorem 6.13 on page 132 establishes conditions for both θ and its truncated versions that guarantee the existence of minimal circulant embeddings for their samples.

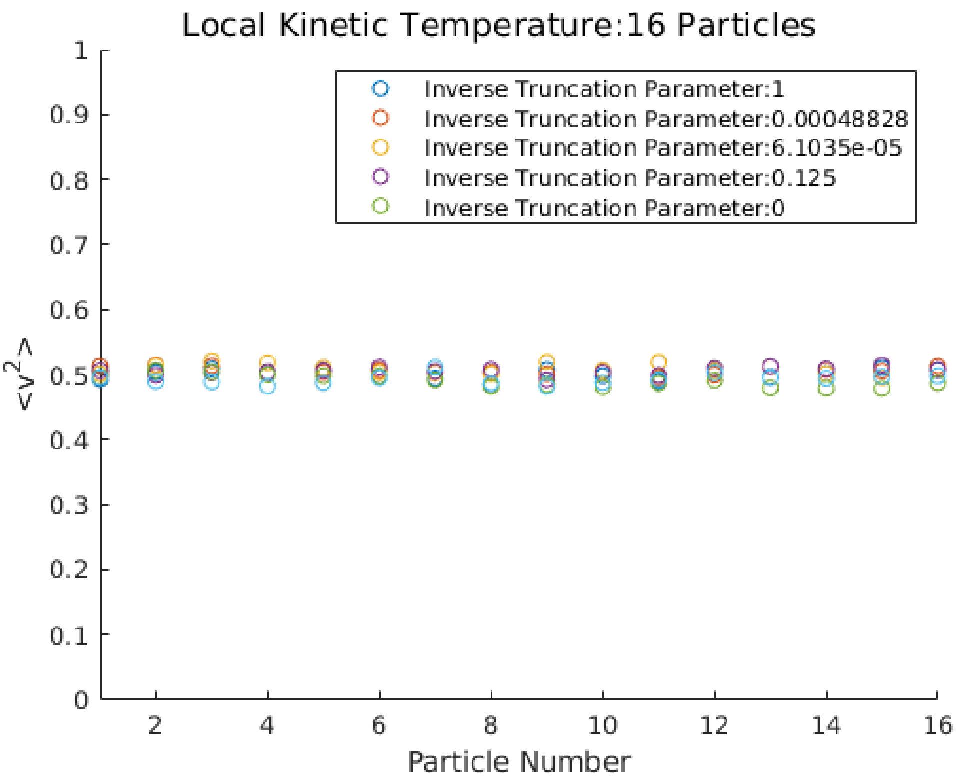
6.3.3 Experiments and Results

Equations 6.9 are simulated where the memory kernel κ is a sum of exponential approximation of either θ or a truncated approximation of the memory kernel, θ_T. Samples of the stationary noise terms are precomputed as outlined in section 6.3.2. The continuous sum of exponentials approximation of the selected memory kernel is also precomputed by first performing a discrete sum of exponentials approximation on a coarse grid with discretization length 0.2.

A third order Runge-Kutta integrator in time is used. At each time step the convolution is computed via the fast convolution for sums of exponentials presented in equation 6.3, where the integral term is approximated with the trapezoidal rule. Samples of the displacements and velocities are recorded every one hundred steps after reaching a pre-defined equilibriation time. Time averages of the observables of interest presented in 1.3 are computed after the simulation has ended. The method is second order accurate in time. Systems of size $N = 2^n, n = 4, \ldots, 10$ particles were selected. Each system size was simulated with bath temperatures $T_L = 0.002, T_R = 0.008$, $T_L = 0.02, T_R = 0.08$, $T_L = 0.2, T_R = 0.8$, $T_L = 0.5, T_R = 0.5$, and $T_L = 2, T_R = 8$. Moreover, for each fixed system size and temperature, simulations performed with an untruncated memory kernel and truncated memory kernels with truncation parameter $T = 2^k, k = 0, \ldots 15$. This resulted in a total of 595 simulations. Each simulation had an final time of $10,000$, an equilibriation time of 5000, and a time step of $\Delta t = 0.001$. The initial conditions had velocities independently and identically sampled from $\mathcal{N}(0, (T_L + T_R)/2)$ normal distributions, while the displacements were sampled uniformly between $(-a/4, a/4)$.

Equilibrium Tests

Simulations with $T_L = T_R = 0.5$ verify no anomalous behavior occurs in the temperature profile when truncated versions of the memory kernel are used. Figure 6.5 beginning on page 138 displays the local kinetic temperature of the system for various system sizes and truncations of the memory kernel. In all of the cases the local kinetic temperature does not exhibit any anomalous behavior at the ends or in the bulk.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Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0
<v^2>
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0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
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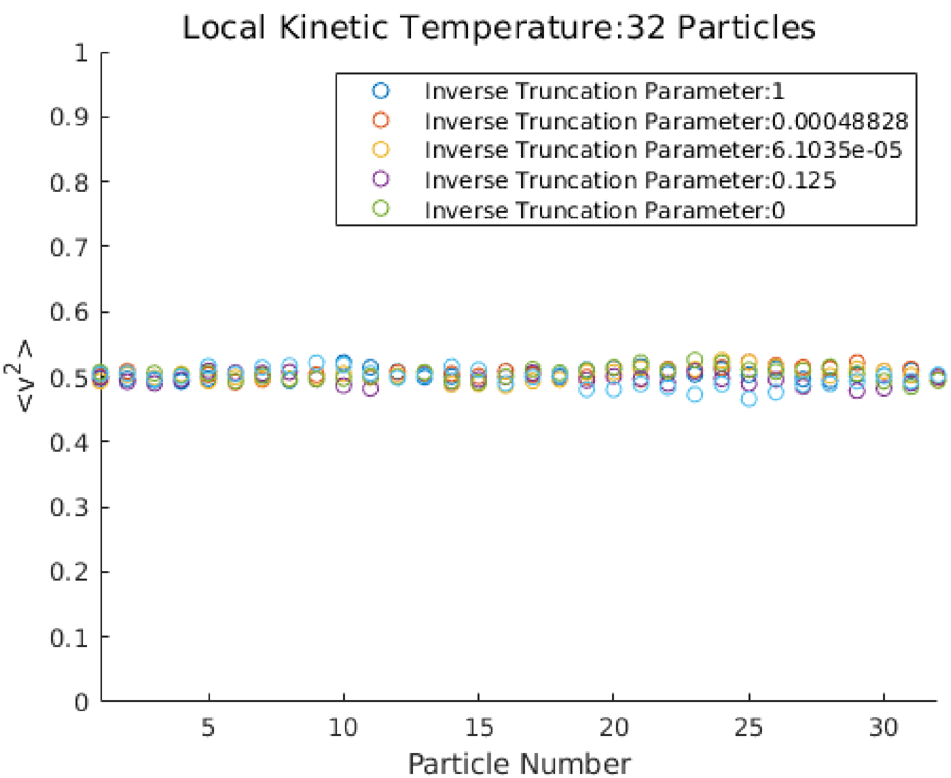
2
4
6
8
10
12
14
16
Particle Number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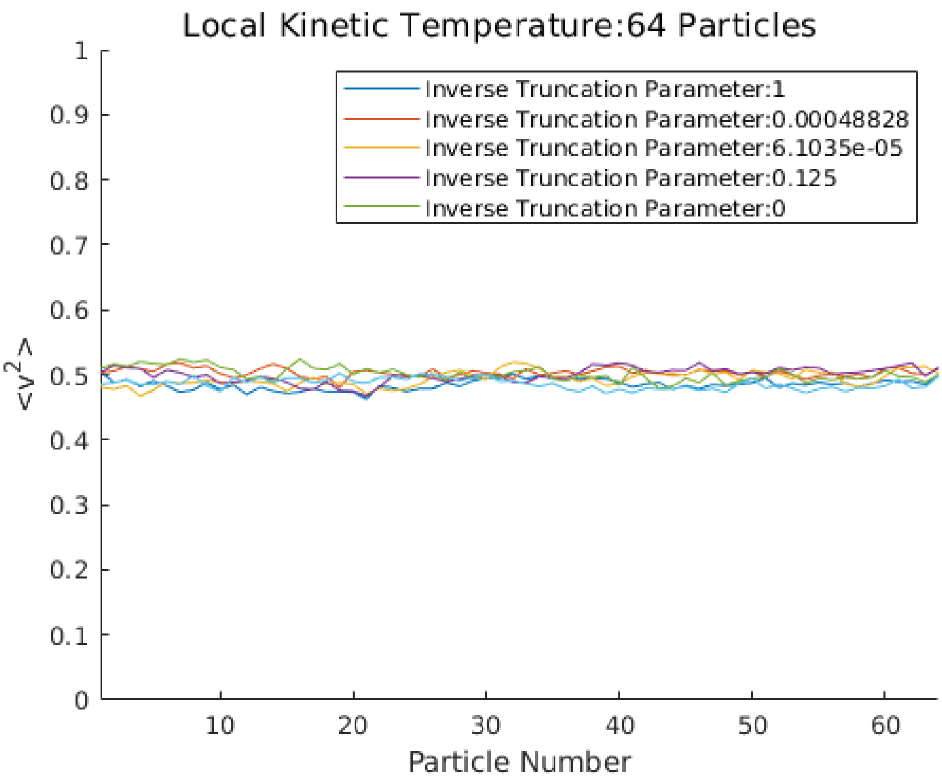
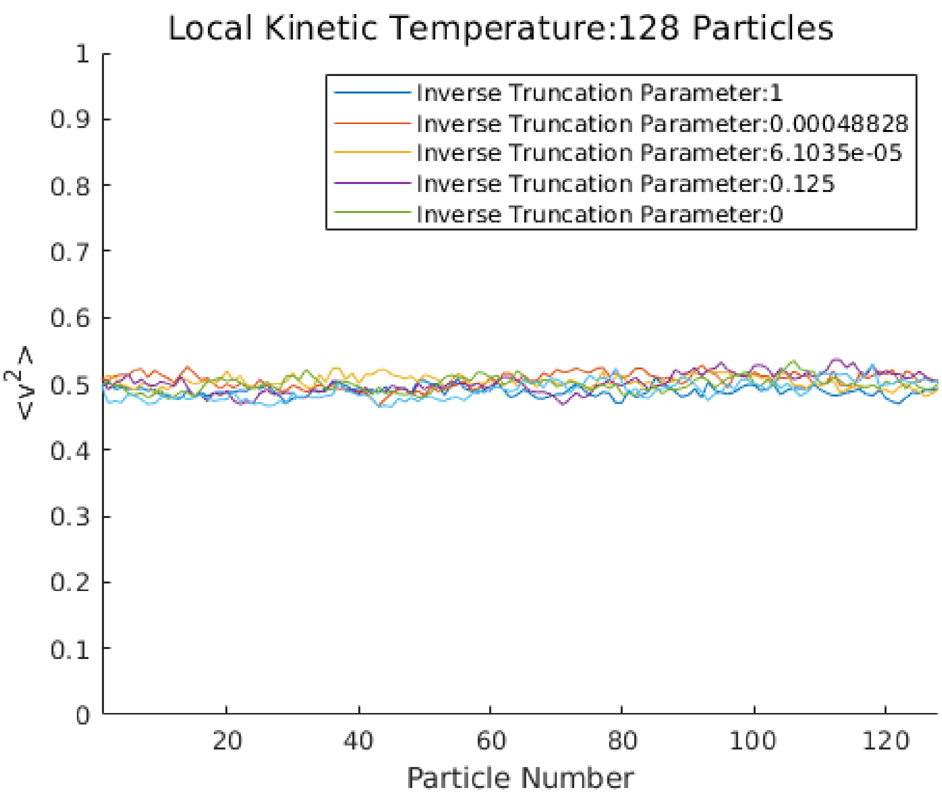
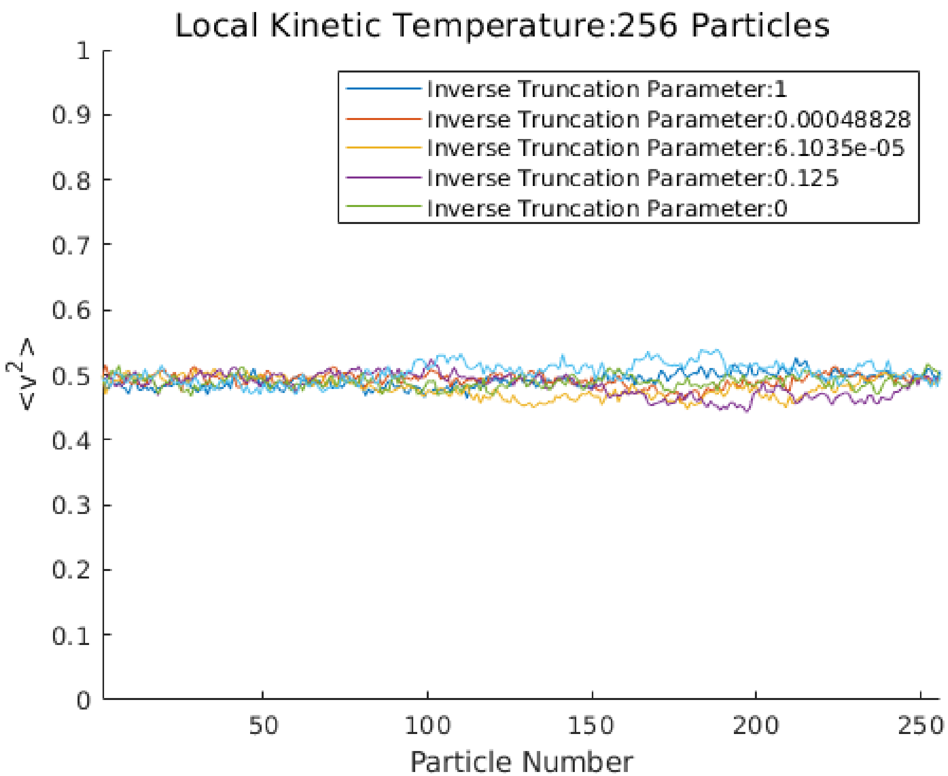
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0
<v^2>
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
5
10
15
20
25
30
Particle Number



Local Kinetic Temperature:64 Particles
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0
<v2>
Particle Number



Local Kinetic Temperature:128 Particles
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0
<v2>
Particle Number


Local Kinetic Temperature:256 Particles
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Inverse Truncation Parameter:0.00048828
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Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0
<v^2>
Particle Number
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
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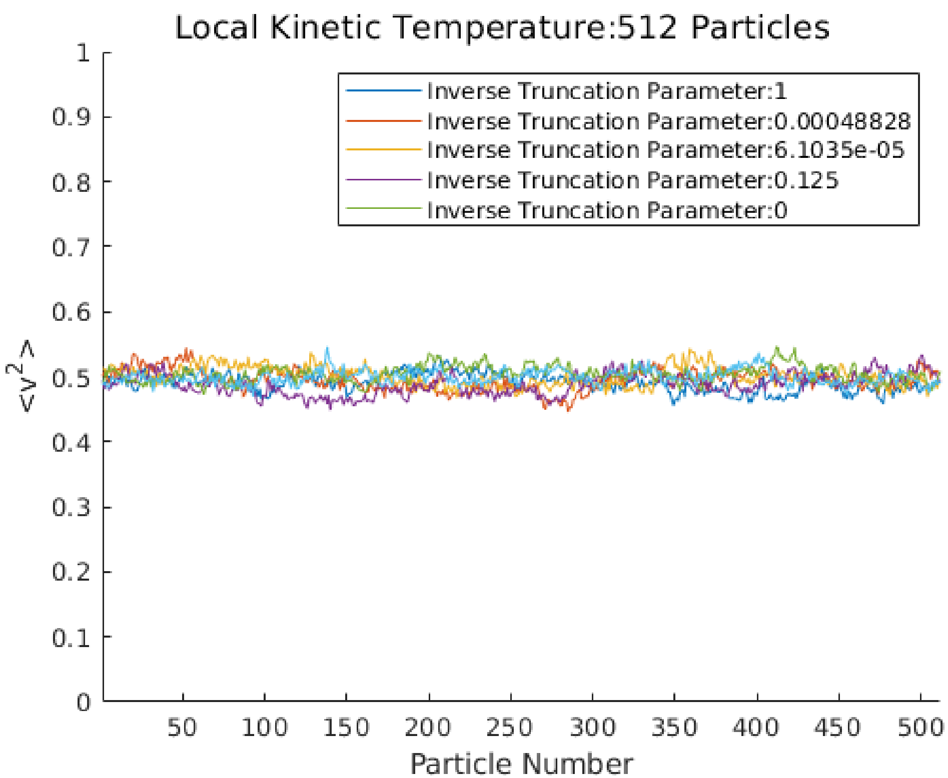
150
200
250


Local Kinetic Temperature:512 Particles
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0
<v^2>
Particle Number
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0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
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150
200
250
300
350
400
450
500

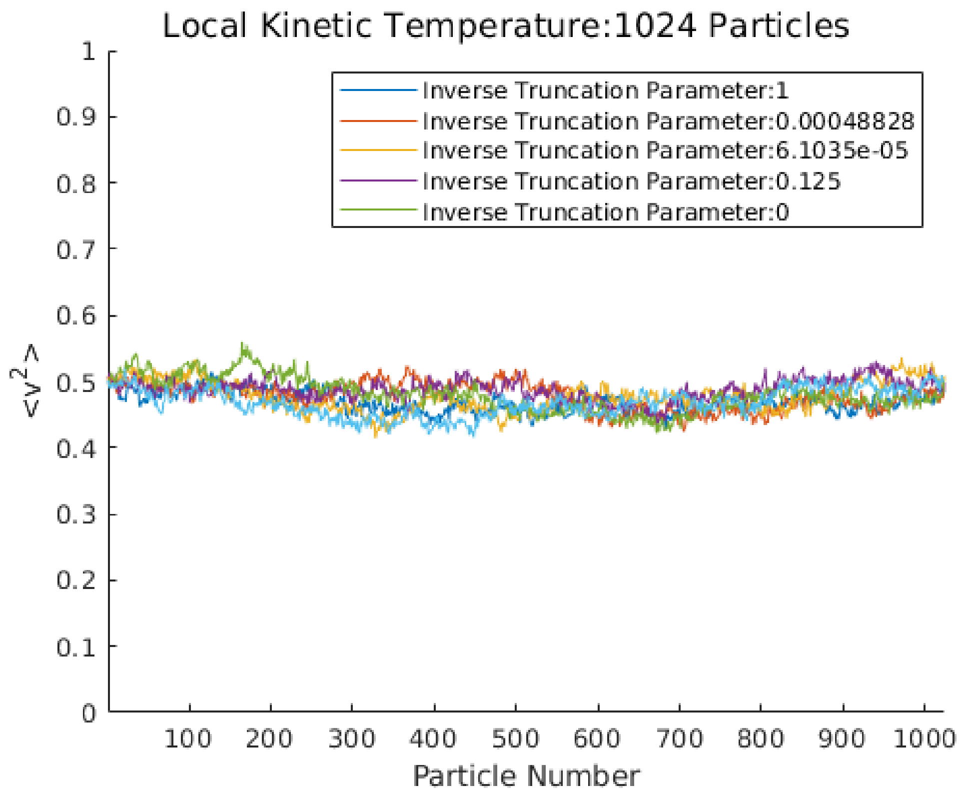


Figure 6.5: Local Kinetic Temperature - Stationary GLE: The inverse truncation parameter is $1/T$ with the convention that $1/\infty = 0$.

Non-Equilibrium Tests

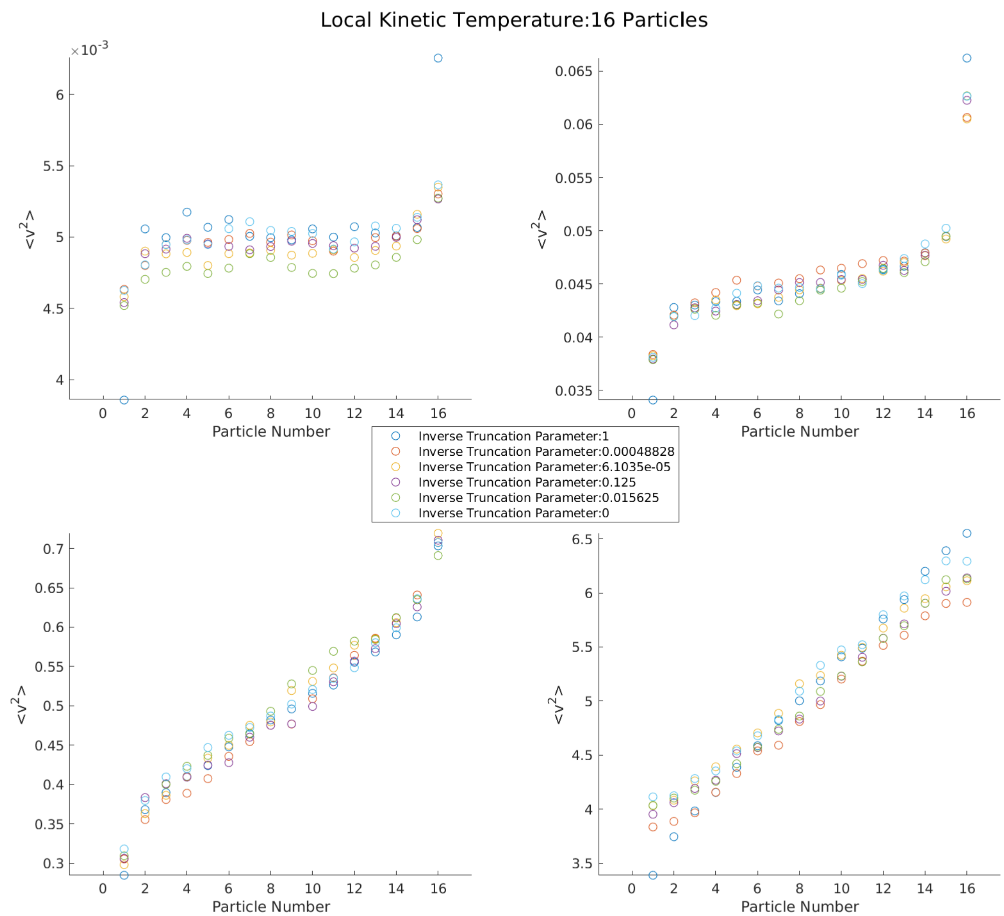
Local Kinetic Temperature: The local kinetic temperature is plotted in Figure 6.6 beginning on page 146. Anomalous behavior for stationary GLE systems is visibly present for all system sizes tested when the temperature difference and average temperature is small. The systems with $T_L = 0.002, T_R = 0.008$ and $T_L = 0.02, T_R = 0.08$ visibly show discontinuities and non-linearities at an near the boundary particles independent of the size of the bath.

The choice of temperature $T_L = 0.002$ and $T_R = 0.008$ have nearly flat temperature profiles in the bulk with sharp discontinuities exactly at the boundary. When the system size increases a slight gradient is visible in the bulk. The local temperature of the boundary particle does not match the selected bath temperatures: The left boundary particle is warmer than the left (colder) bath while the right is cooler than the right (hotter) bath. The size of the discontinuity measured from the bulk seems to increase with the truncation size. A larger discontinuity forms at the interface when the truncations become more extreme. However that means that the difference of the empirical local temperature of the boundary particles from the selected bath temperatures increases when there is less truncation of the memory kernel.

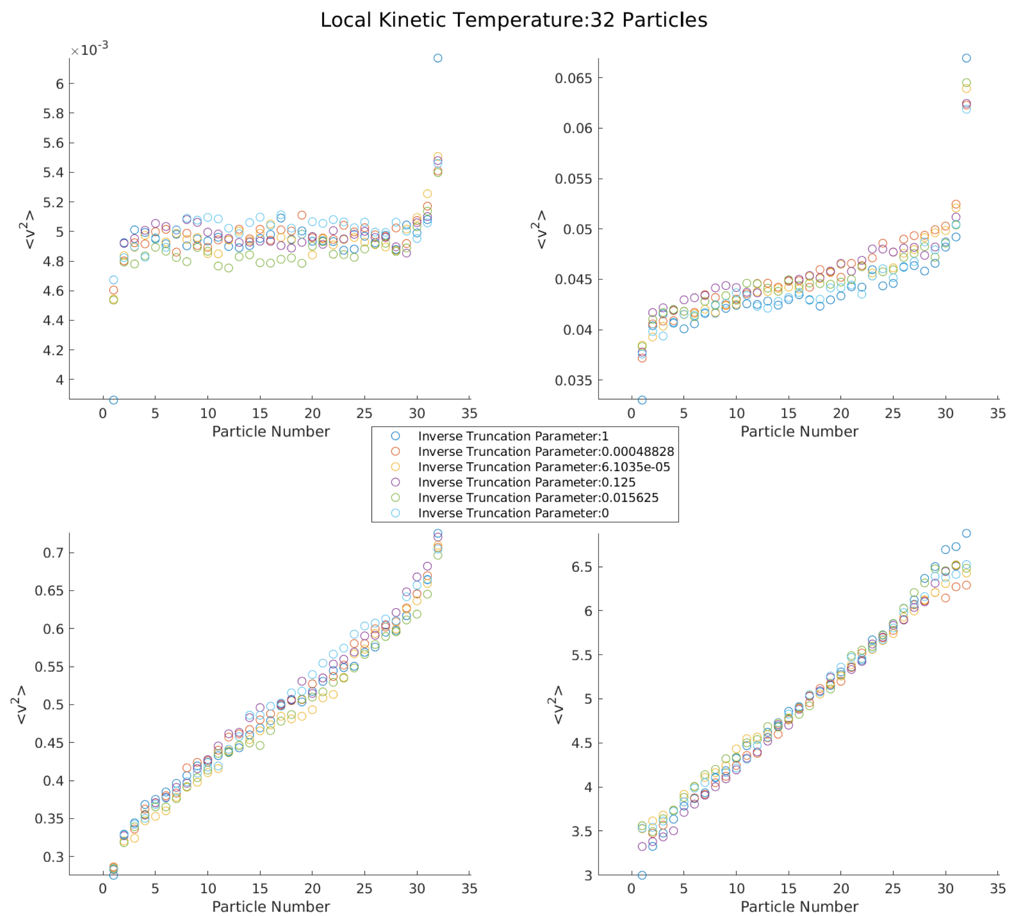
Increasing the temperature to $T_L = 0.02$ and $T_R = 0.08$ reduces the strength of the anomalous behavior in the local temperature. While the bulk now experiences a clear linear profile, there is a strong nonlinear effect near the boundary which is more pronounced for small systems and more extreme truncations. Again the local temperature at the boundaries is not near the selected bath temperatures.

When the temperatures are $T_L = 0.2$ and $T_R = 0.8$ the anomalous behavior is further reduced. At these choices of temperatures there is no longer a discontinuity or severe nonlinearity near the boundaries. The local temperature has a clear linear profile in the bulk which slightly bends when approaching the interfaces. When the total number of particles is greater than or equal to 512, the boundary particles local temperature match the selected temperature, while for smaller systems the boundary particles fail to meet the selected temperatures.

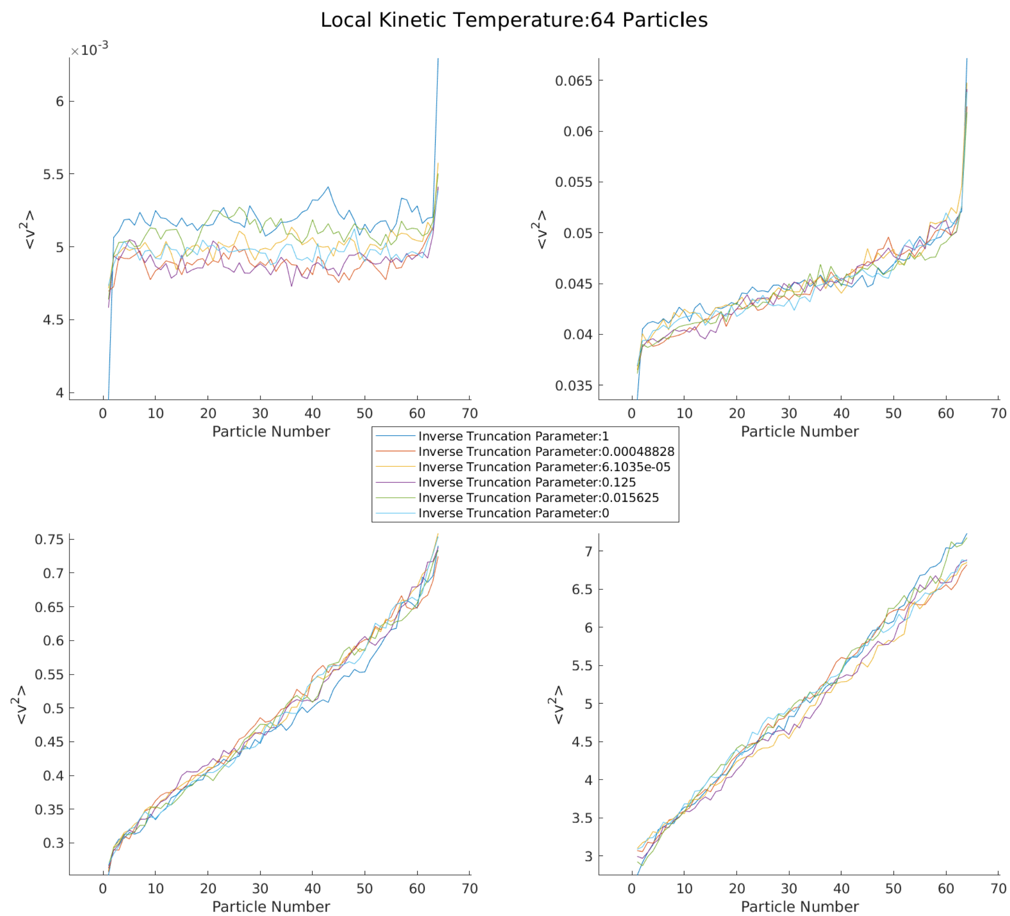
Finally when selecting the bath temperatures to be $T_L = 2$ and $T_R = 8$ the temperature profile of all the systems is almost entirely linear throughout irregardless of truncation size or system size, with only mild nonlinearity near the interface. Contrary to the previous temperature selection, the only system which managed to have its boundary particle's local temperature meet the selected temperatures was the system of size 1024.



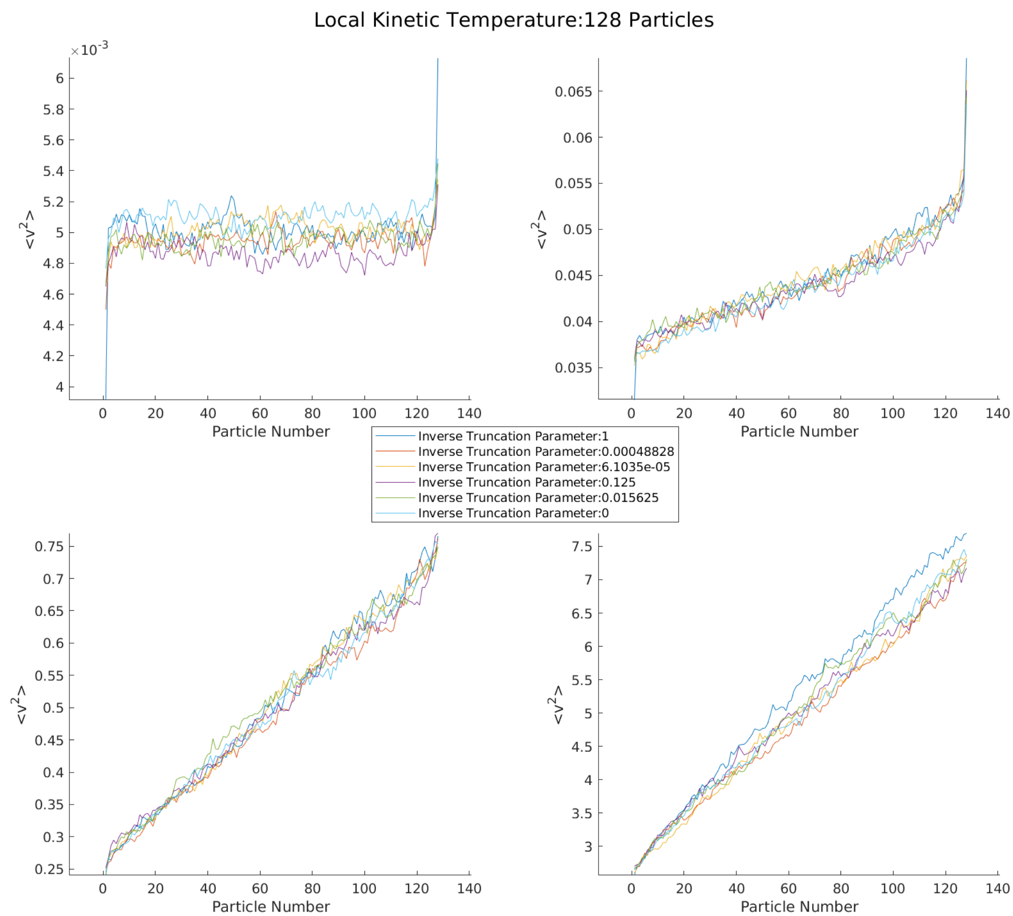
Local Kinetic Temperature:16 Particles
×10-3
<v2>
Particle Number
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0.015625
Inverse Truncation Parameter:0



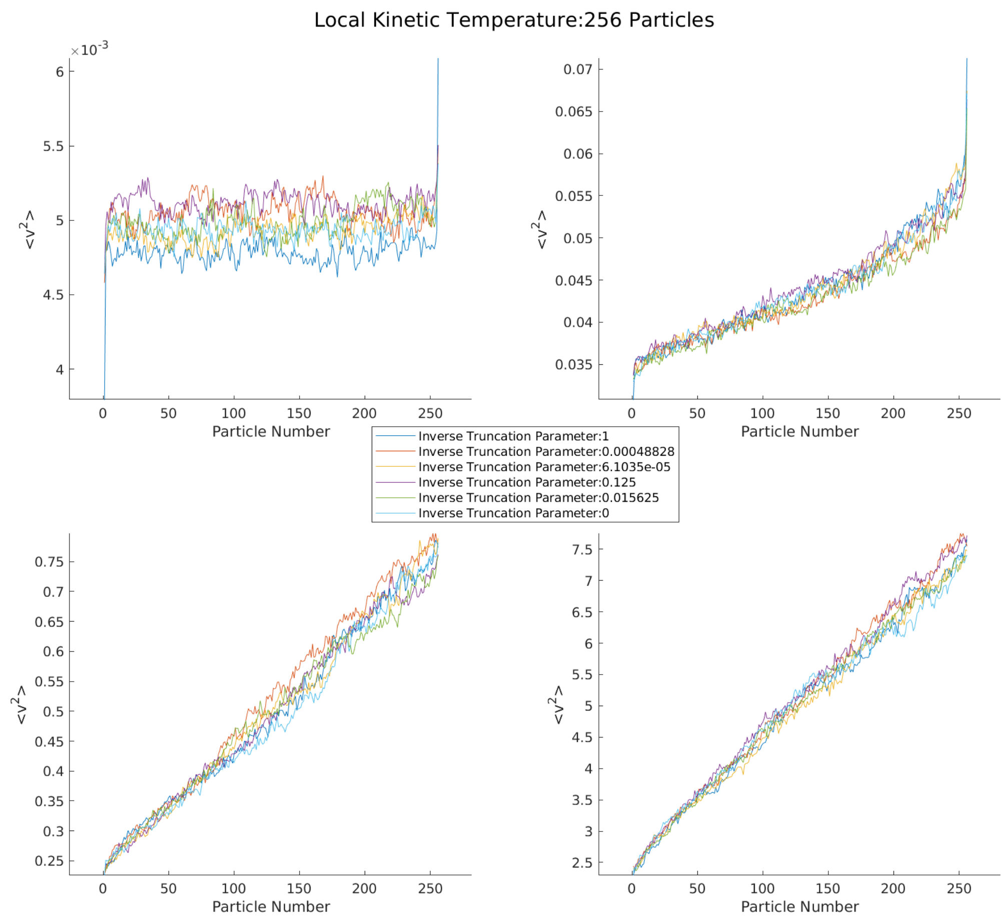
Local Kinetic Temperature:32 Particles
<v^2>
Particle Number
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0.015625
Inverse Truncation Parameter:0



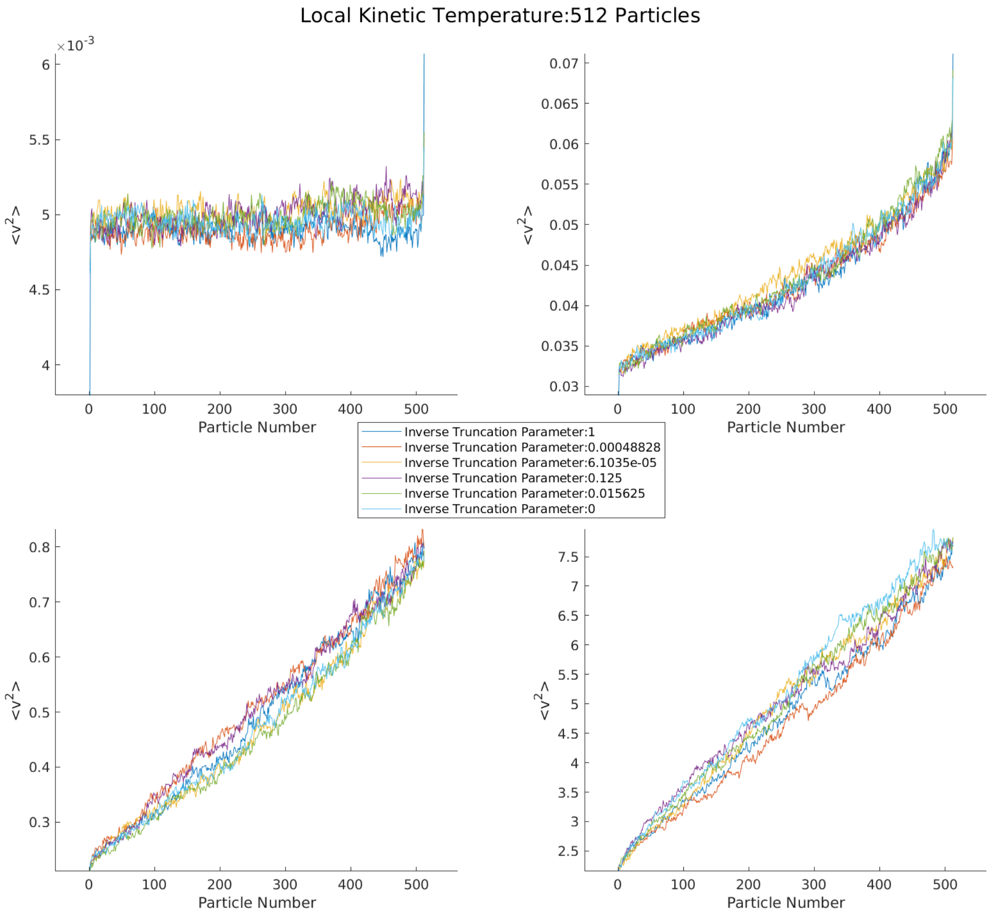
Local Kinetic Temperature:64 Particles
Particle Number
<v^2>
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0.015625
Inverse Truncation Parameter:0



Local Kinetic Temperature:128 Particles
Particle Number
<v^2>
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0.015625
Inverse Truncation Parameter:0



Local Kinetic Temperature:256 Particles
<v2>
Particle Number
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0.015625
Inverse Truncation Parameter:0


Local Kinetic Temperature:512 Particles
<v^2>
Particle Number
Inverse Truncation Parameter:1
Inverse Truncation Parameter:0.00048828
Inverse Truncation Parameter:6.1035e-05
Inverse Truncation Parameter:0.125
Inverse Truncation Parameter:0.015625
Inverse Truncation Parameter:0

T_L - T_R	α	α°	$\alpha^\circ - \alpha$
0.002 - 0.008	1.9598	1.9611	1.3×10^{-3}
0.02 - 0.08	1.702	1.7035	1.5×10^{-3}
0.2 - 0.8	1.3314	1.3319	5×10^{-4}
2 - 8	1.1861	1.1940	7.9×10^{-3}

Table 6.2: Heat Conductivity Scaling - Stationary GLE

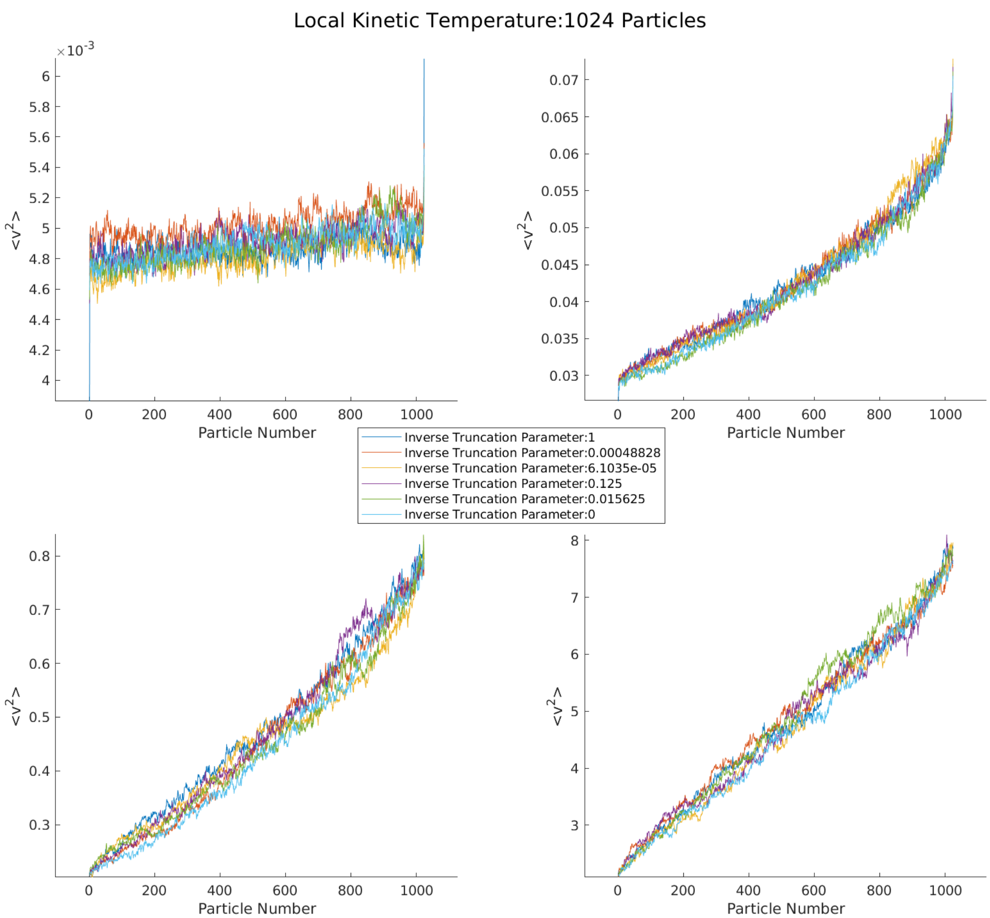
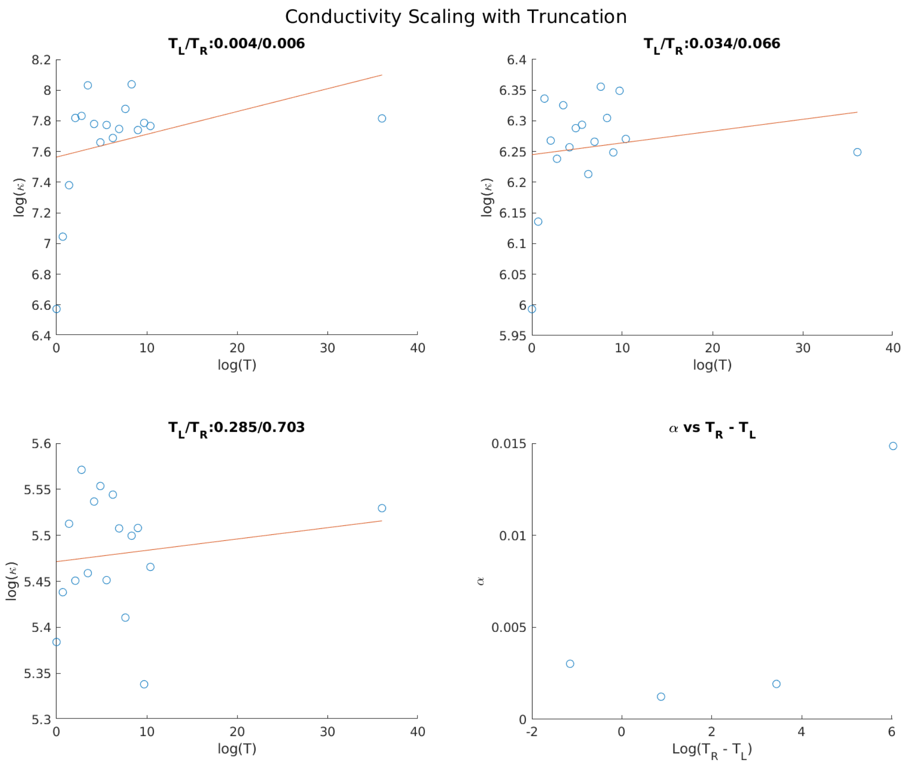
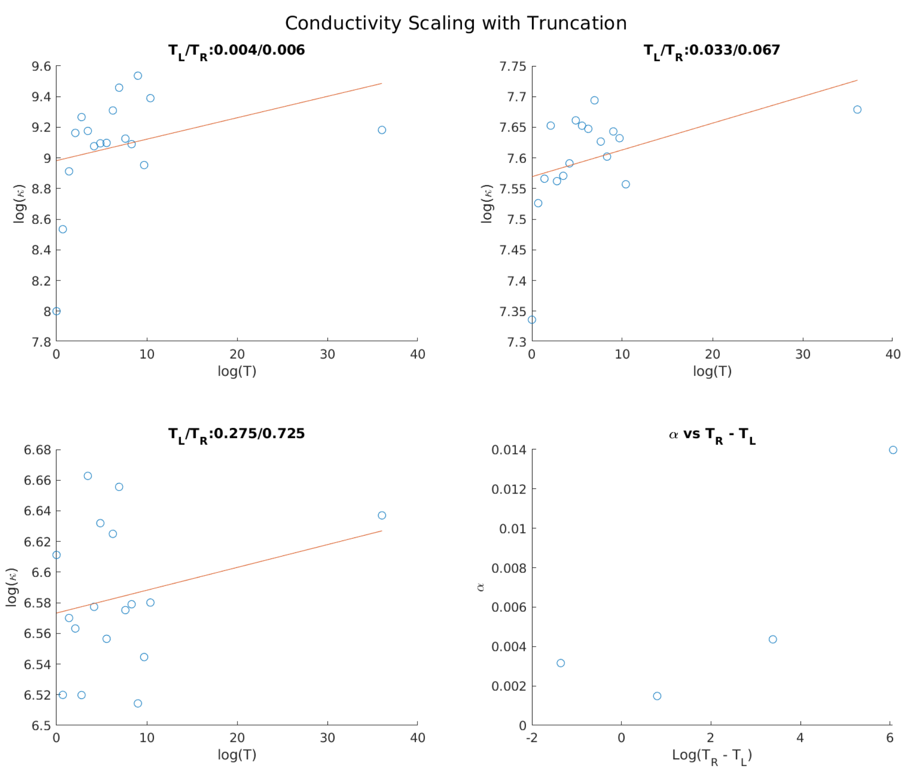
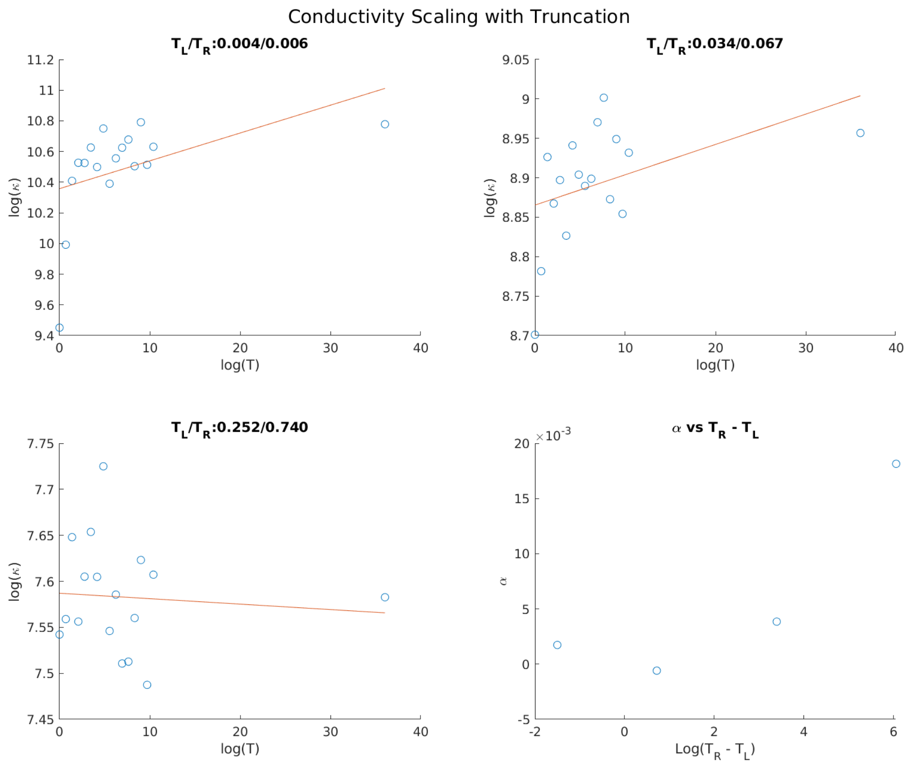


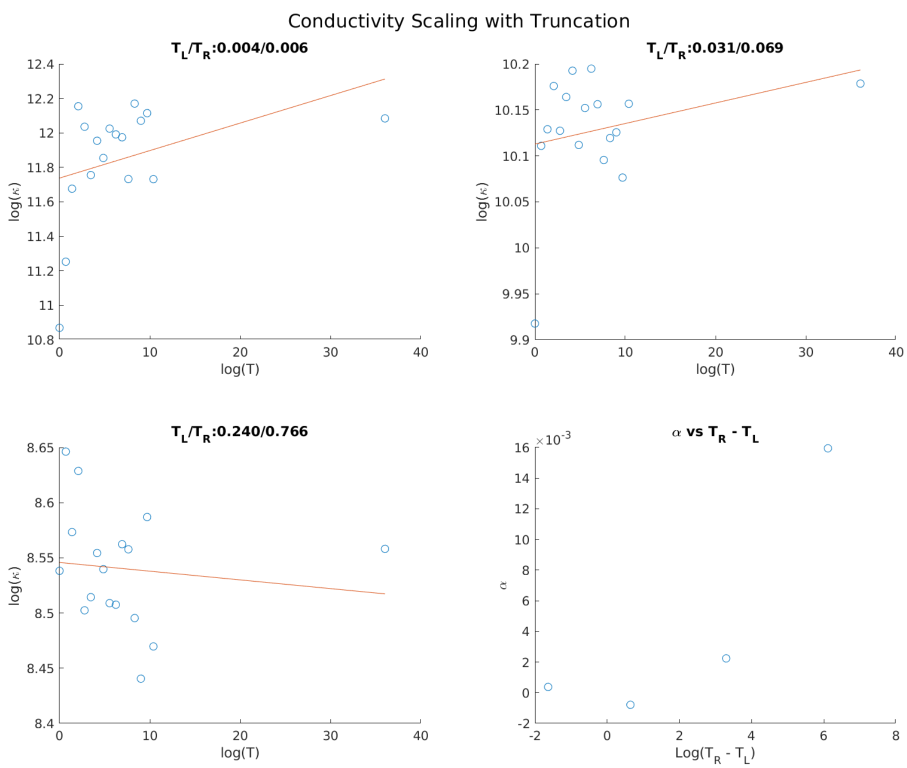
Figure 6.6: Local Kinetic Temperature - Stationary GLE: The inverse truncation parameter is $1/T_c$ with the convention that $1/\infty = 0$.

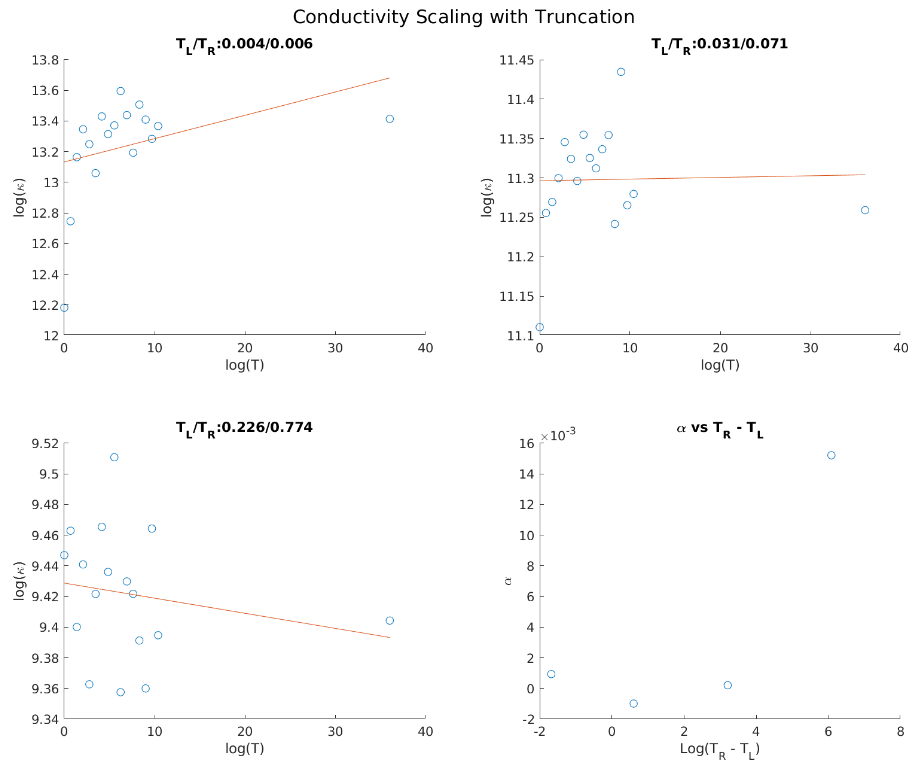
Conductivity Scaling Figure 6.7 beginning on page 185 plots $\log(\kappa)$ and $\log(\kappa^\circ)$ as a function of $\log(N)$. The linearity present in the log-log plot indicates that κ and κ° scale as N^α and N^{α^o} respectively. As seen in Table 6.2 on page 146, for the stationary GLE system, α and α° are nearly the same, with differences on the order of 10^{-3}, indicating that small oscillations of the system do not have a strong impact on the divergence of the conductivity when stationarity of the noise is assumed. As the temperature difference and average temperature is increased the conductivity scaling coefficients decrease, however their positivity indicates that heat flow is anomalous and does not obey Fourier's law. Built into the construction of the truncated versions of the memory kernels, the Green-Kubo relations were enforced [4]. This normalizes the thermal transport coefficients of the truncated versions of the memory kernel to be the same as the untruncated memory kernel. Thus we should expect little to no scaling of κ and κ^{o} with T. In figures 6.8 and 6.9 beginning on pages 151 and 155 respectively we show various plots comparing κ and κ° to the truncation parameter T. On all the systems investigated the values of the scaling parameter β and β^{o} have order of magnitude at most 10^{-2} and can be positive or negative. Figures 6.10 and 6.11 beginning on pages 159 and 162 respectively plots β and β^{o} vs $\log(T_R - T_L)$, more easily show behavior.

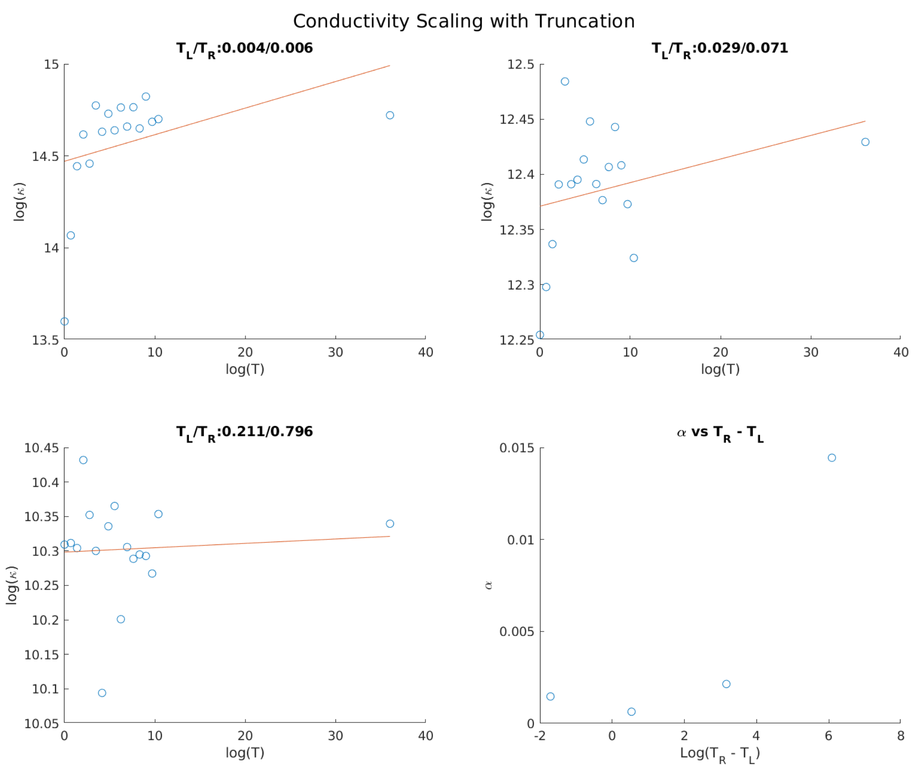

Conductivity Scaling with Truncation
T_L/T_R:0.004/0.006
T_L/T_R:0.034/0.066
T_L/T_R:0.285/0.703
α vs T_R - T_L
log(κ)
log(T)
α
Log(T_R - T_L)


Conductivity Scaling with Truncation
T_L/T_R:0.004/0.006
T_L/T_R:0.033/0.067
T_L/T_R:0.275/0.725
α vs T_R - T_L
log(κ)
log(T)
α
Log(T_R - T_L)


Conductivity Scaling with Truncation
T_L/T_R:0.004/0.006
T_L/T_R:0.034/0.067
T_L/T_R:0.252/0.740
α vs T_R - T_L
log(κ)
log(T)
α
Log(T_R - T_L)


Conductivity Scaling with Truncation
T_L/T_R:0.004/0.006
T_L/T_R:0.031/0.069
T_L/T_R:0.240/0.766
α vs T_R - T_L
log(κ)
log(T)
α
Log(T_R - T_L)


Conductivity Scaling with Truncation
T_L/T_R:0.004/0.006
T_L/T_R:0.031/0.071
T_L/T_R:0.226/0.774
α vs T_R - T_L
log(κ)
log(T)
α
Log(T_R - T_L)


Conductivity Scaling with Truncation
T_L/T_R:0.004/0.006
T_L/T_R:0.029/0.071
T_L/T_R:0.211/0.796
α vs T_R - T_L
log(κ)
log(T)
α
Log(T_R - T_L)

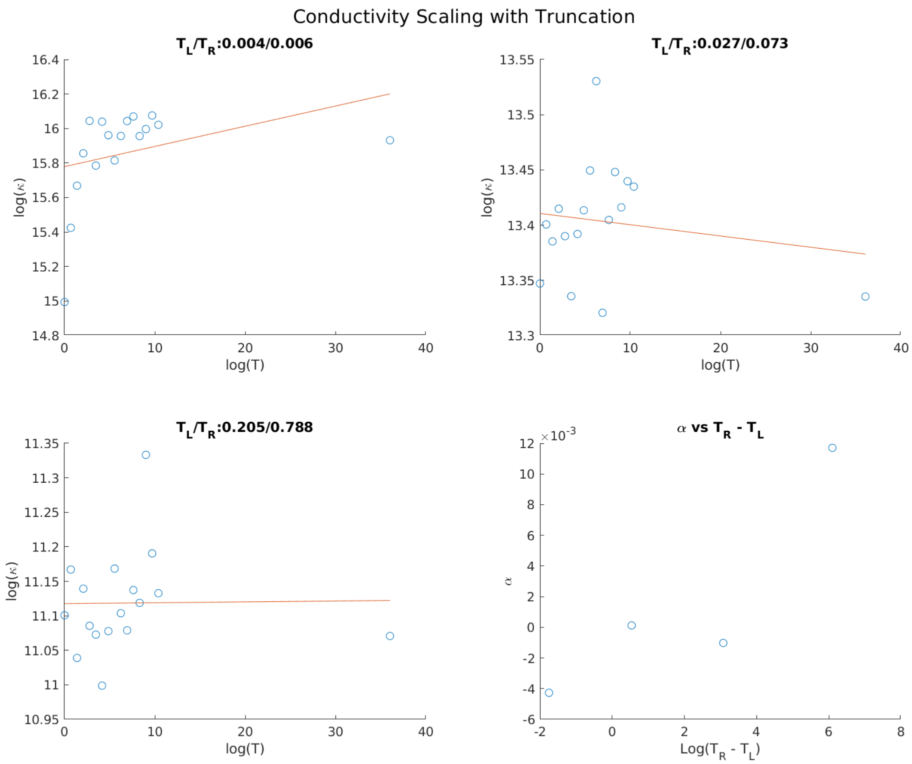
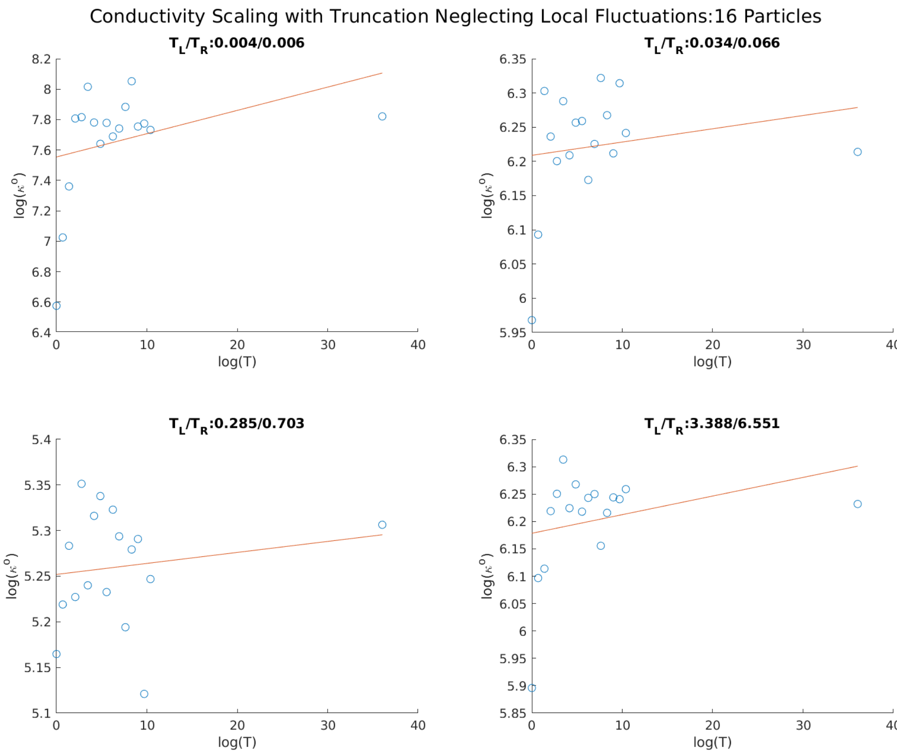
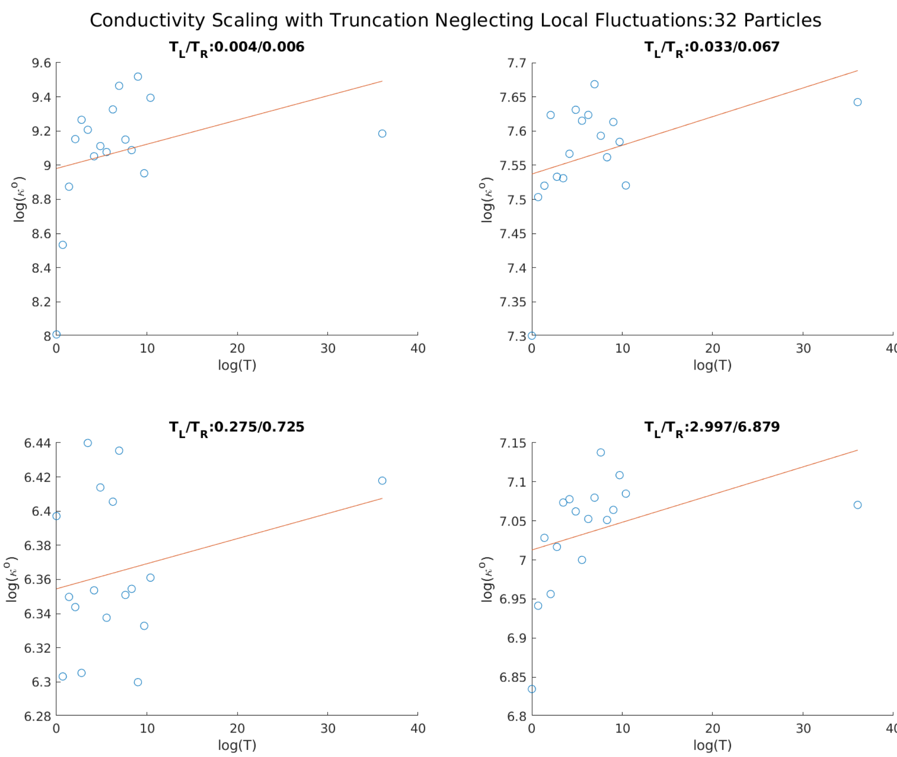
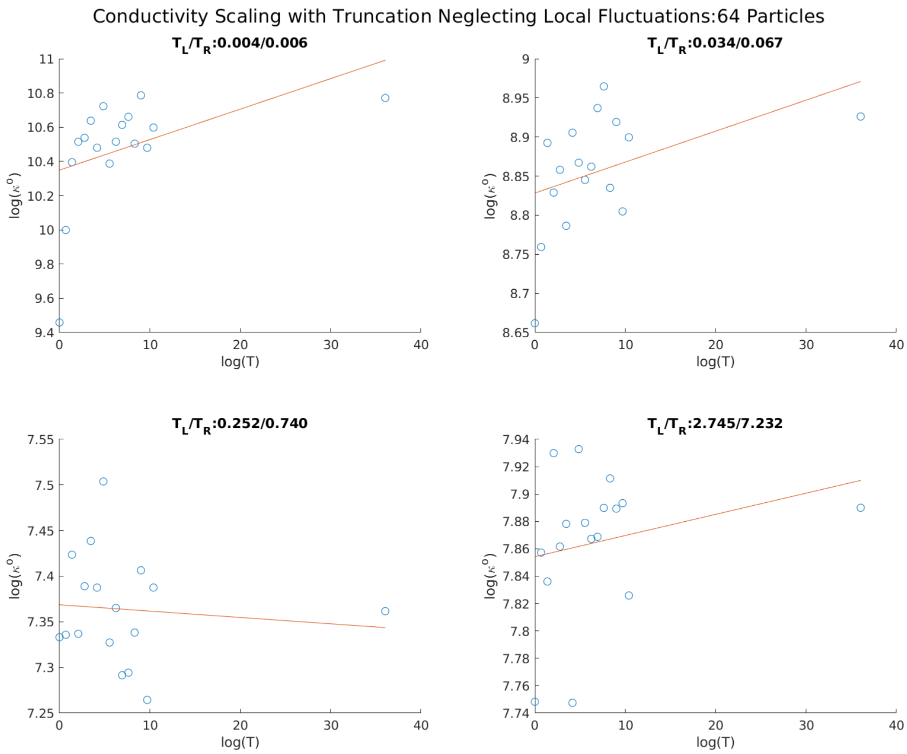


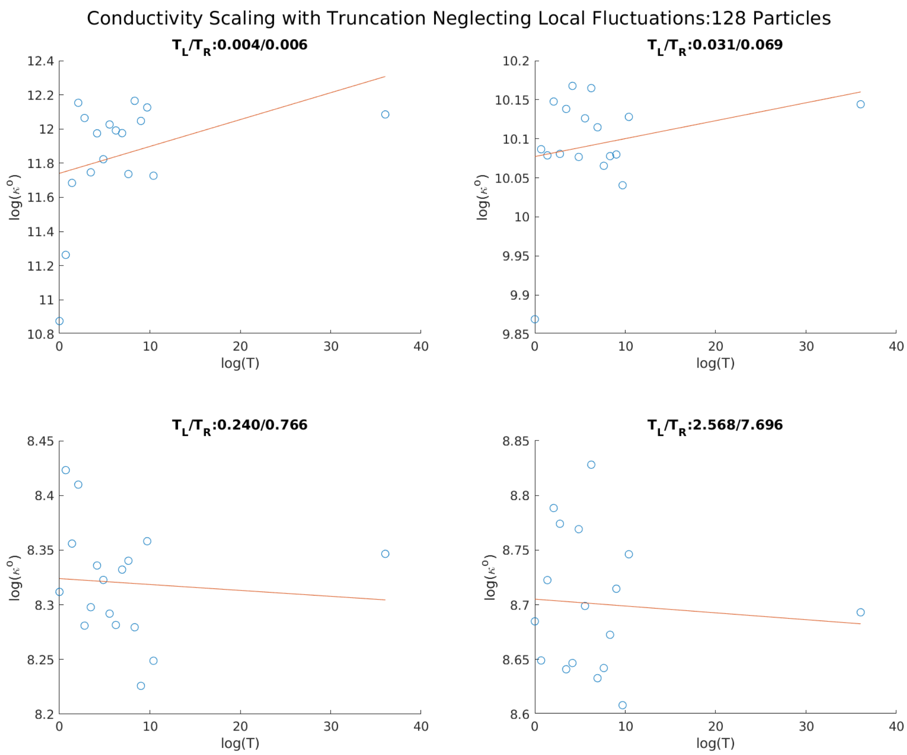
Figure 6.8: κ vs $\log T$ - Stationary GLE: $\log(\kappa)$ does not appear to scale with the log truncation parameter, $\log(T)$ at any temperature or system size. The slope of the best fit line is β


Conductivity Scaling with Truncation Neglecting Local Fluctuations:16 Particles
T_L/T_R:0.004/0.006
T_L/T_R:0.034/0.066
T_L/T_R:0.285/0.703
T_L/T_R:3.388/6.551
log(κ^o)
log(T)

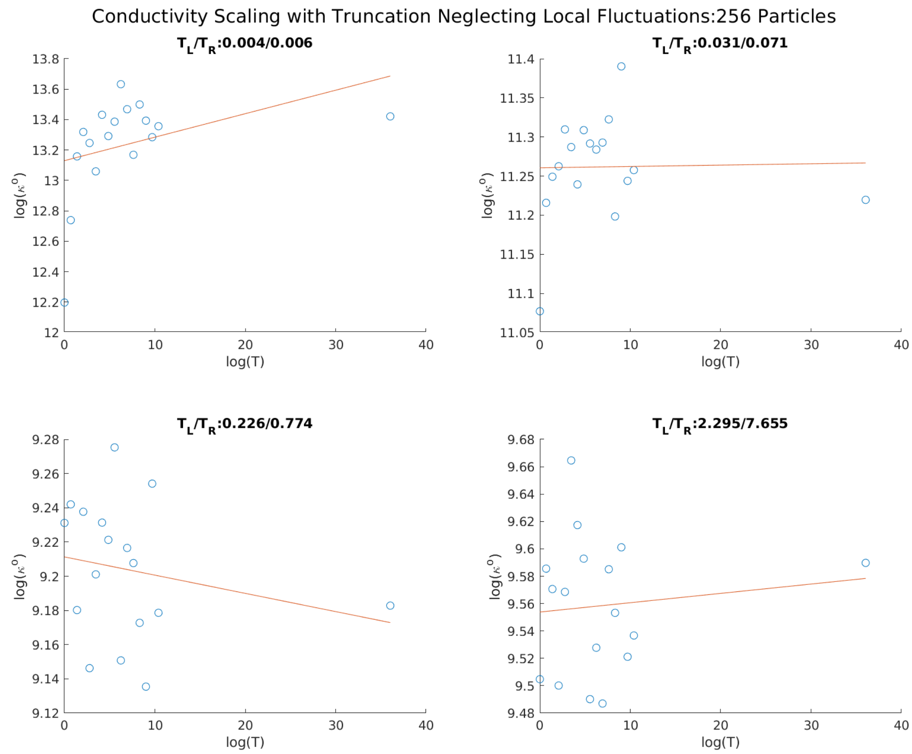

Conductivity Scaling with Truncation Neglecting Local Fluctuations:32 Particles
T_L/T_R:0.004/0.006
T_L/T_R:0.033/0.067
T_L/T_R:0.275/0.725
T_L/T_R:2.997/6.879
log(κ^o)
log(T)

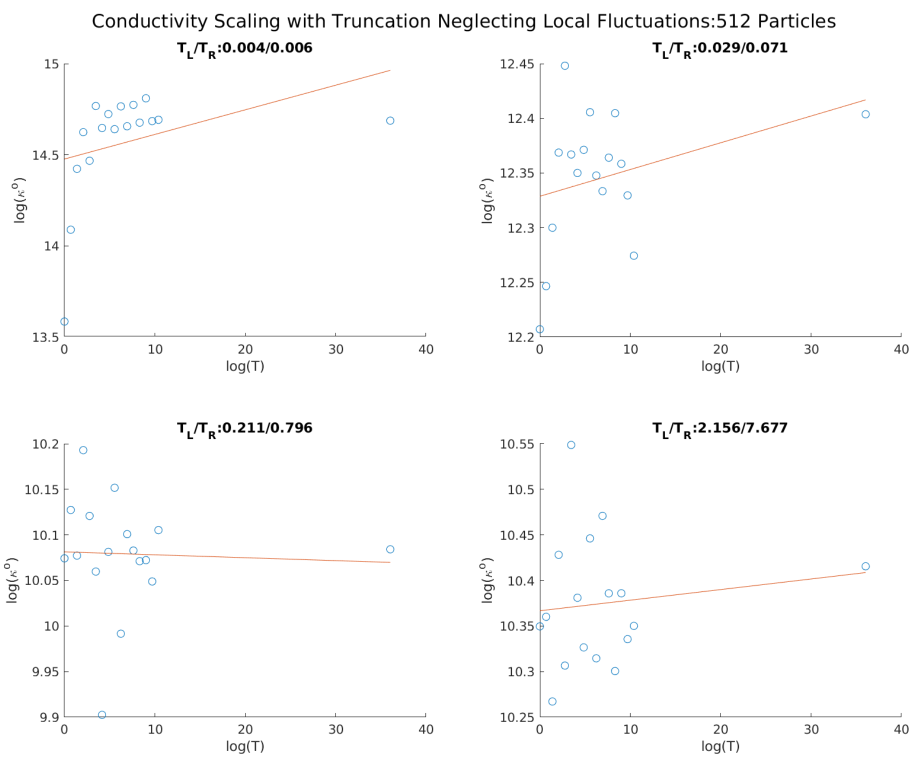


Conductivity Scaling with Truncation Neglecting Local Fluctuations:64 Particles
T_L/T_R:0.004/0.006
T_L/T_R:0.034/0.067
T_L/T_R:0.252/0.740
T_L/T_R:2.745/7.232
log(κ^0)
log(T)



Conductivity Scaling with Truncation Neglecting Local Fluctuations:128 Particles
T_L/T_R:0.004/0.006
T_L/T_R:0.031/0.069
T_L/T_R:0.240/0.766
T_L/T_R:2.568/7.696
log(κ^0)
log(T)


Conductivity Scaling with Truncation Neglecting Local Fluctuations:256 Particles
T_L/T_R:0.004/0.006
T_L/T_R:0.031/0.071
T_L/T_R:0.226/0.774
T_L/T_R:2.295/7.655
$\log(\kappa^0)$
log(T)


Conductivity Scaling with Truncation Neglecting Local Fluctuations:512 Particles
T_L/T_R:0.004/0.006
T_L/T_R:0.029/0.071
T_L/T_R:0.211/0.796
T_L/T_R:2.156/7.677
$\log(\kappa^0)$
log(T)

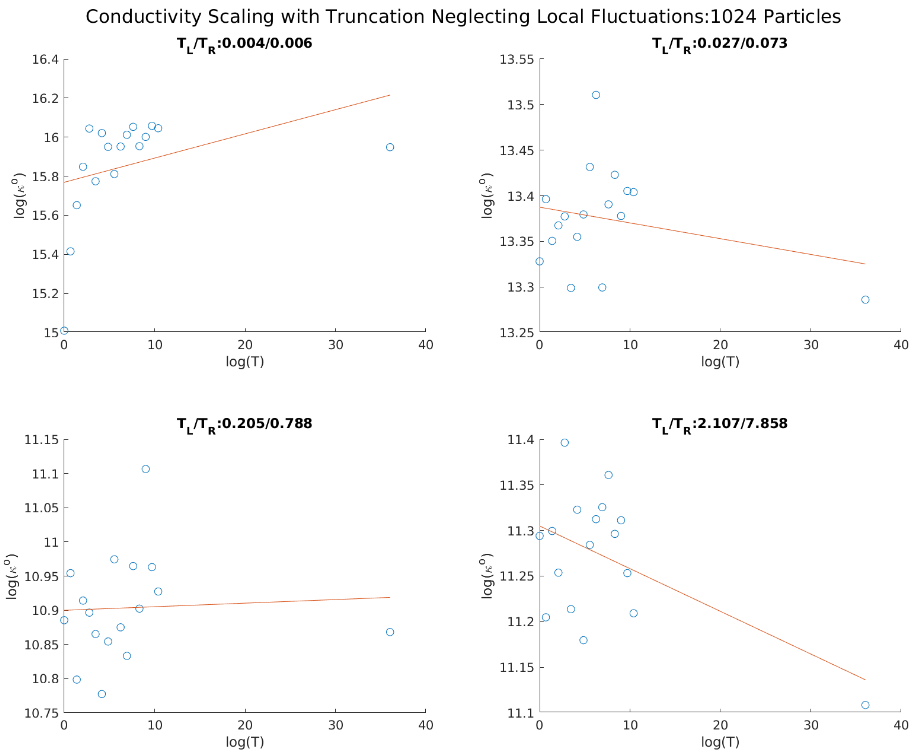
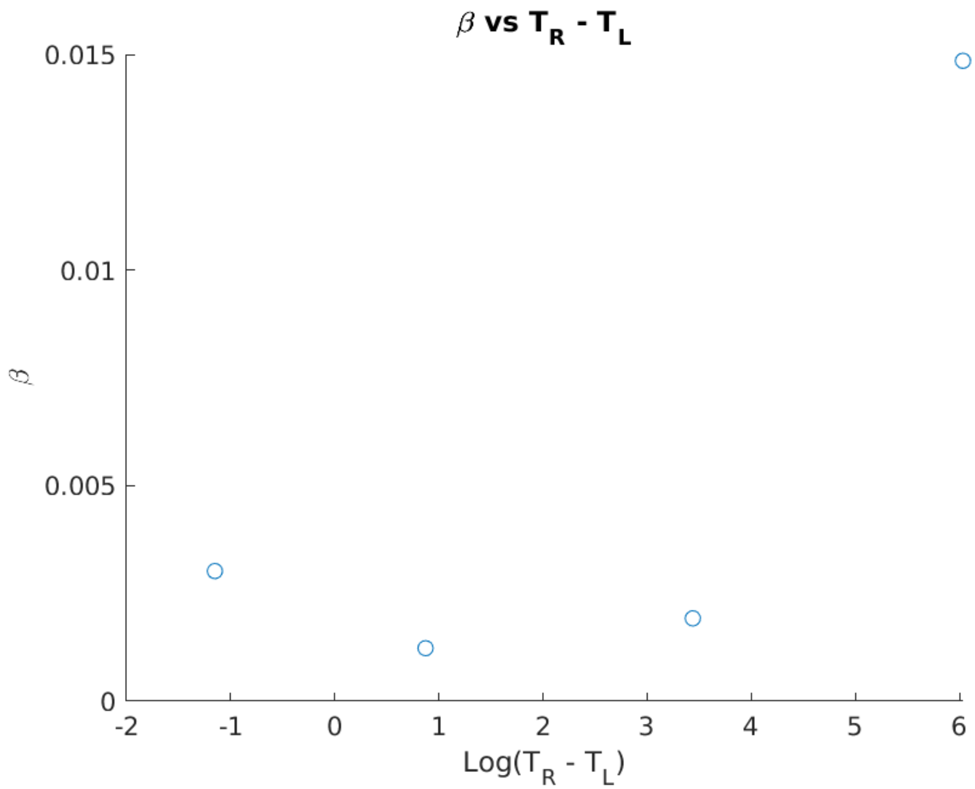
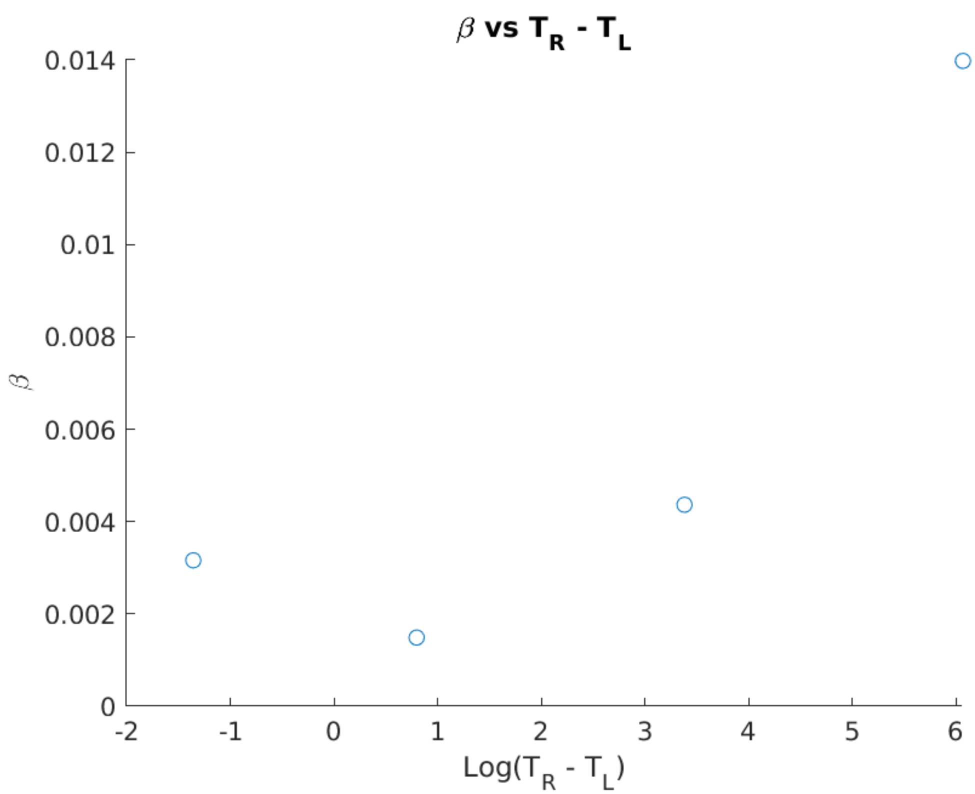
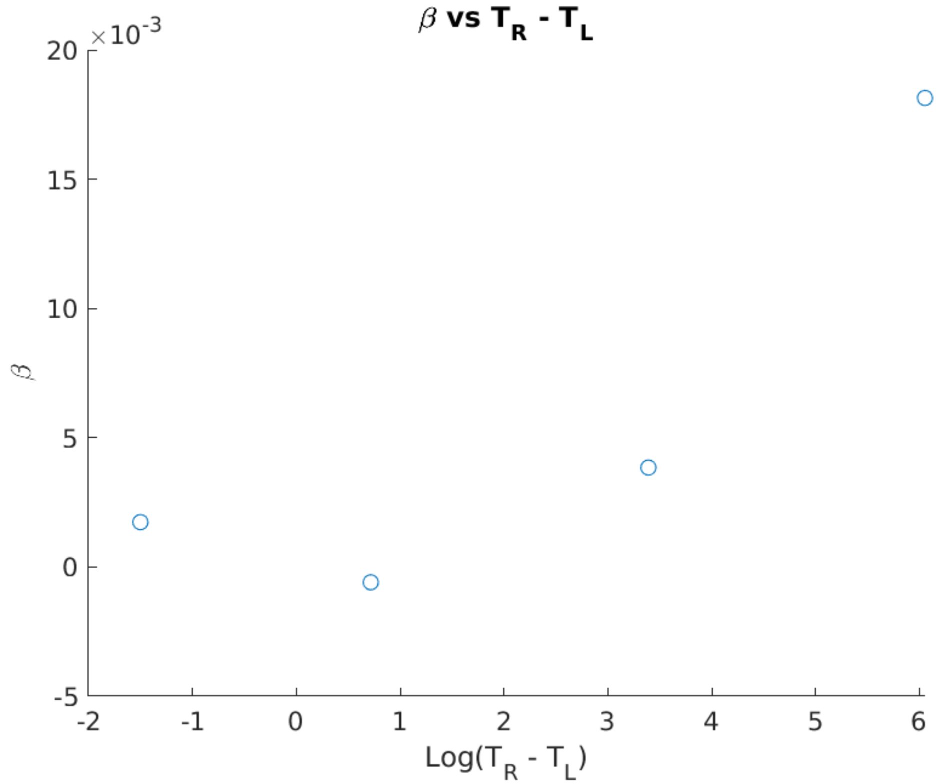
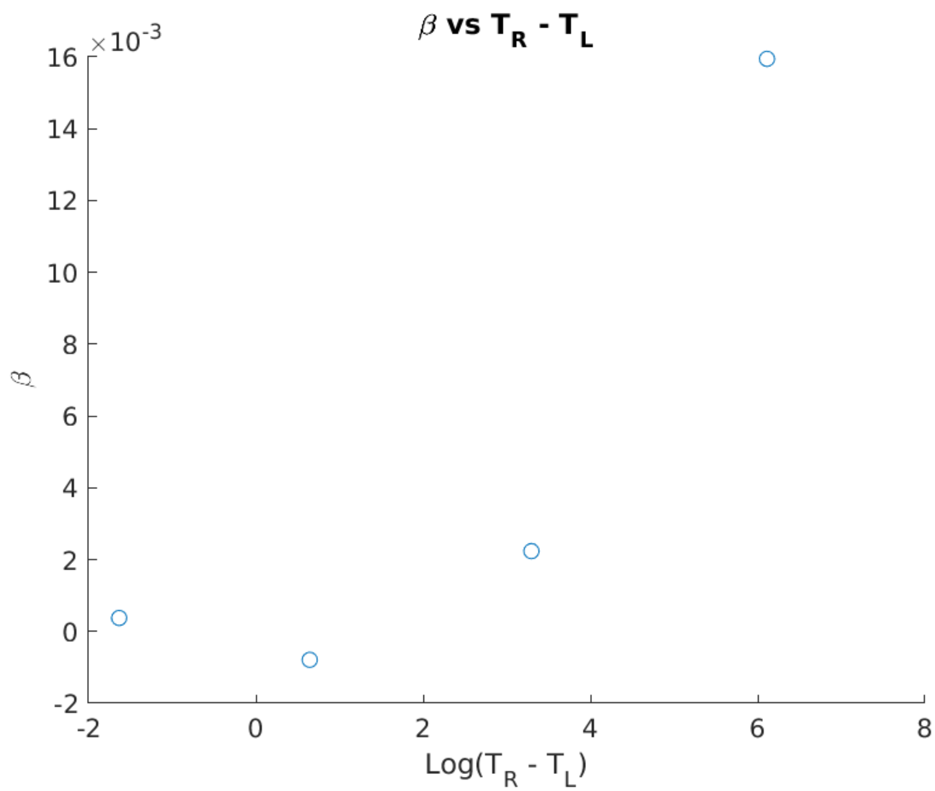


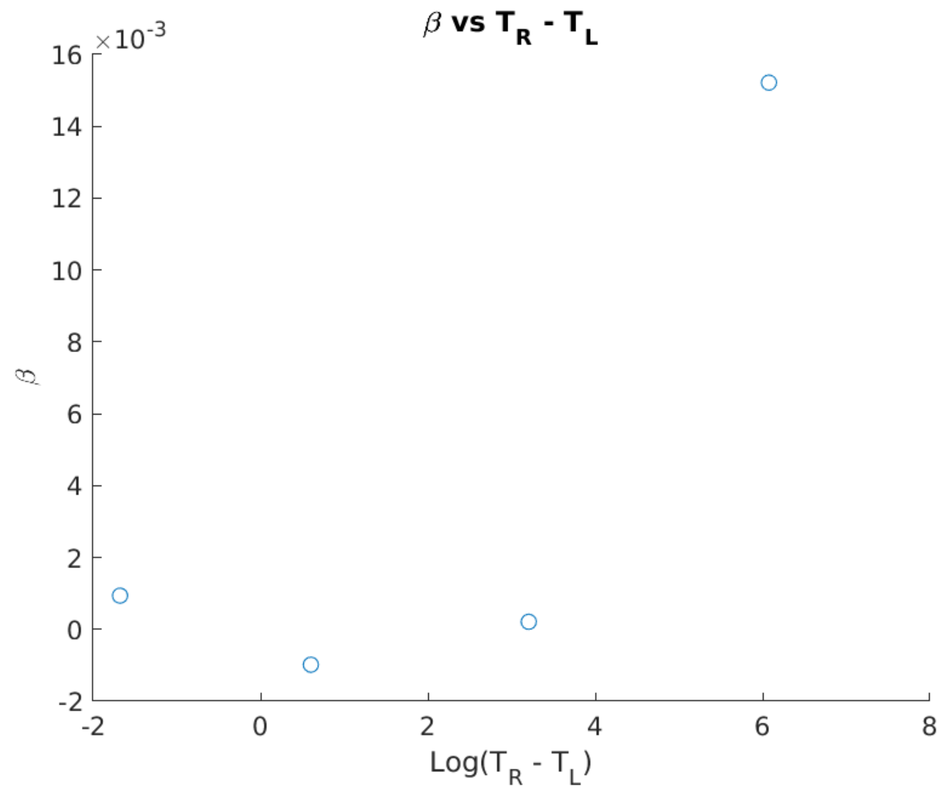
Figure 6.9: κ^o vs $\log T$ - Stationary GLE: $\log(\kappa^o)$ does not appear to scale with the log truncation parameter, $\log(T)$ at any temperature or system size. The slope of the best fit line is β^o

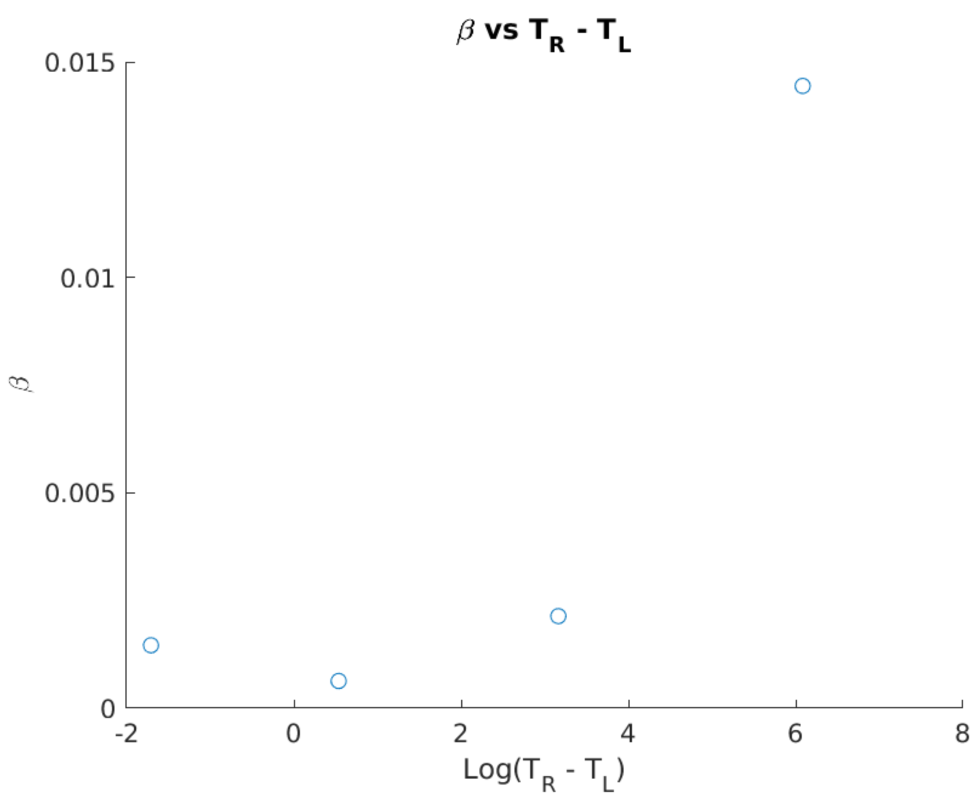

β vs T_R - T_L
0.015
0.01
0.005
0
β
-2
-1
0
1
2
3
4
5
6
Log(T_R - T_L)


β vs T_R - T_L
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
β
-2
-1
0
1
2
3
4
5
6
Log(T_R - T_L)


β vs T_R - T_L
$\times 10^{-3}$
20
15
10
5
0
-5
β
-2
-1
0
1
2
3
4
5
6
$Log(T_R - T_L)$


β vs T_R - T_L
$\times 10^{-3}$
16
14
12
10
8
6
4
2
0
-2
β
-2
0
2
4
6
8
$Log(T_R - T_L)$


β vs T_R - T_L
$\times 10^{-3}$
16
14
12
10
8
6
4
2
0
-2
β
-2
0
2
4
6
8
Log(T_R - T_L)


β vs T_R - T_L
0.015
0.01
0.005
0
β
-2
0
2
4
6
8
Log(T_R - T_L)

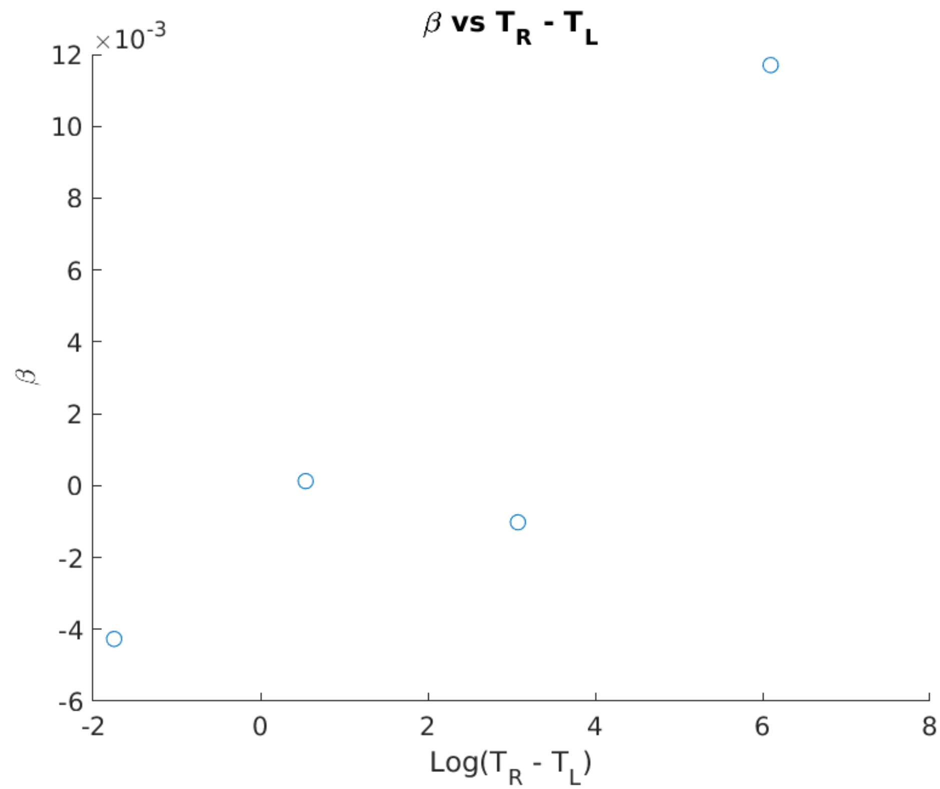
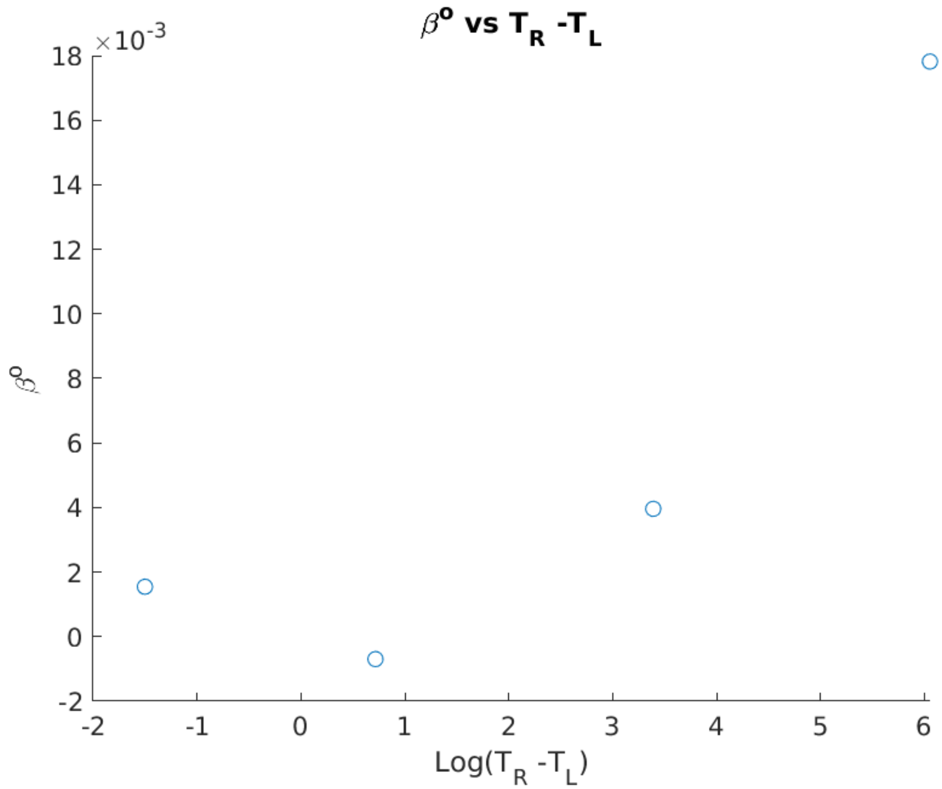
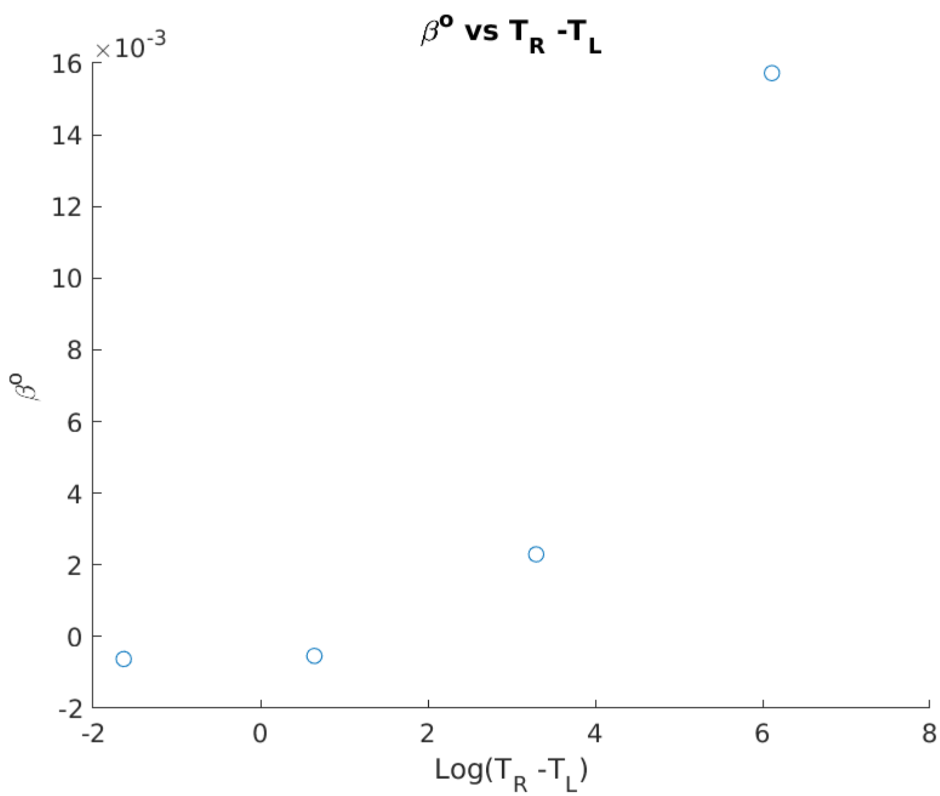


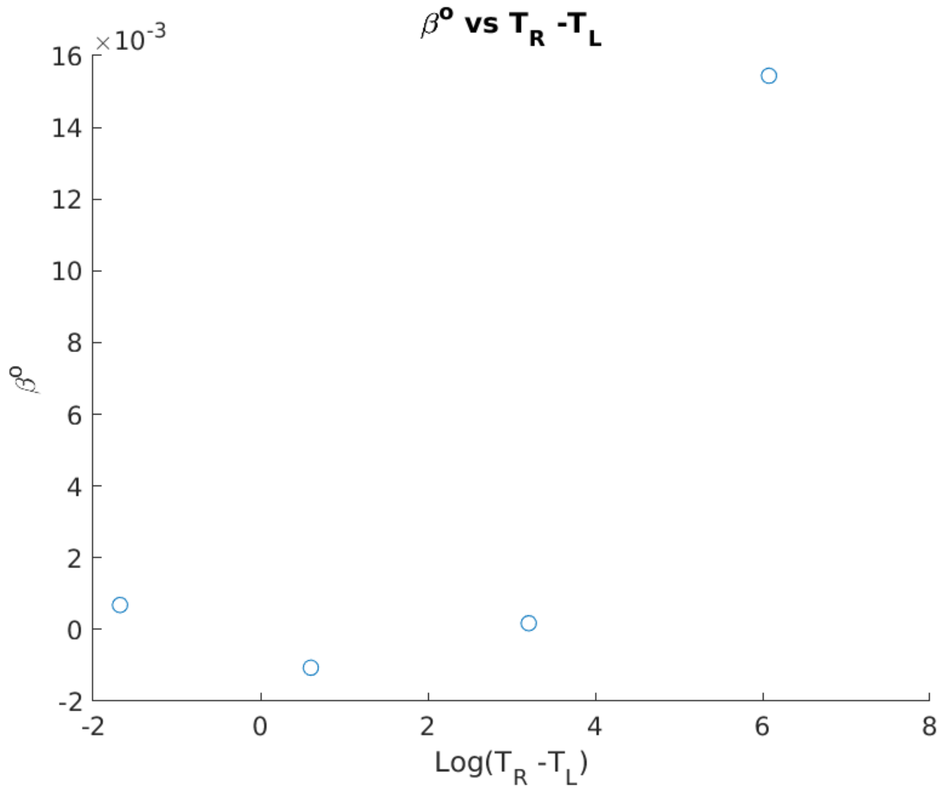
Figure 6.10: β vs $T_R - T_L$ - Stationary GLE: β does not appear to depend strongly on $T_R - T_L$.

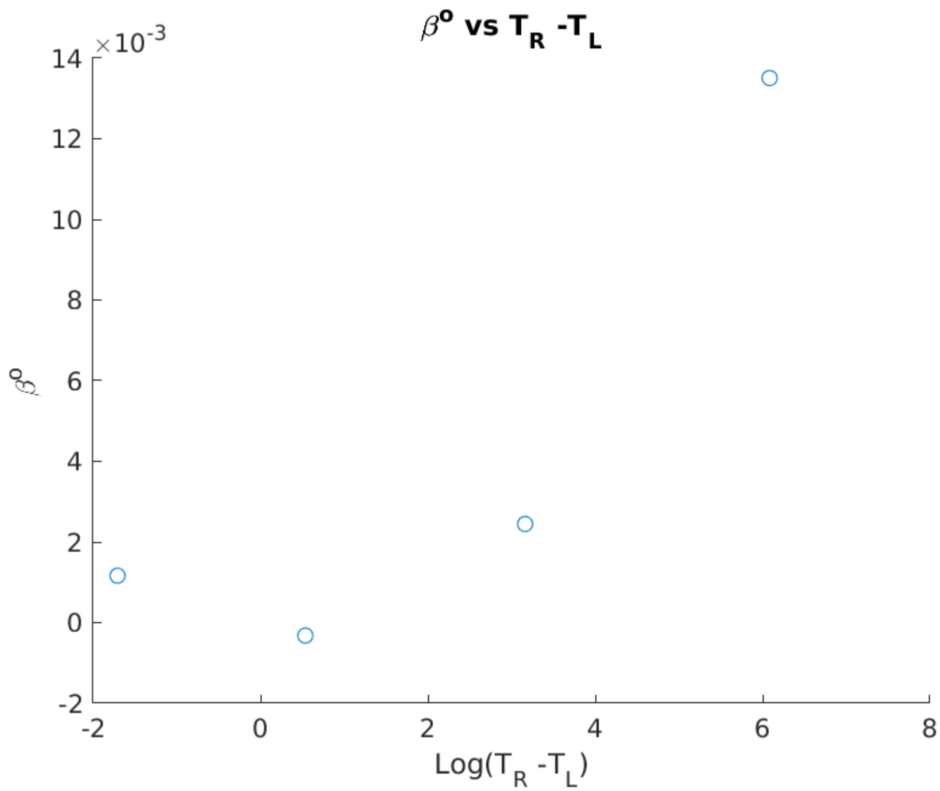


β^o vs T_R -T_L
$\times 10^{-3}$
18
16
14
12
10
8
6
4
2
0
-2
β^o
-2
-1
0
1
2
3
4
5
6
Log(T_R -T_L)



β^o vs T_R -T_L
$\times 10^{-3}$
16
14
12
10
8
6
4
2
0
-2
β^o
-2
0
2
4
6
8
Log(T_R -T_L)


β^o vs T_R -T_L
$\times 10^{-3}$
16
14
12
10
8
6
4
2
0
-2
β^o
-2
0
2
4
6
8
Log(T_R -T_L)


β^o vs T_R -T_L
$\times 10^{-3}$
14
12
10
8
6
4
2
0
-2
β^o
-2
0
2
4
6
8
Log(T_R -T_L)

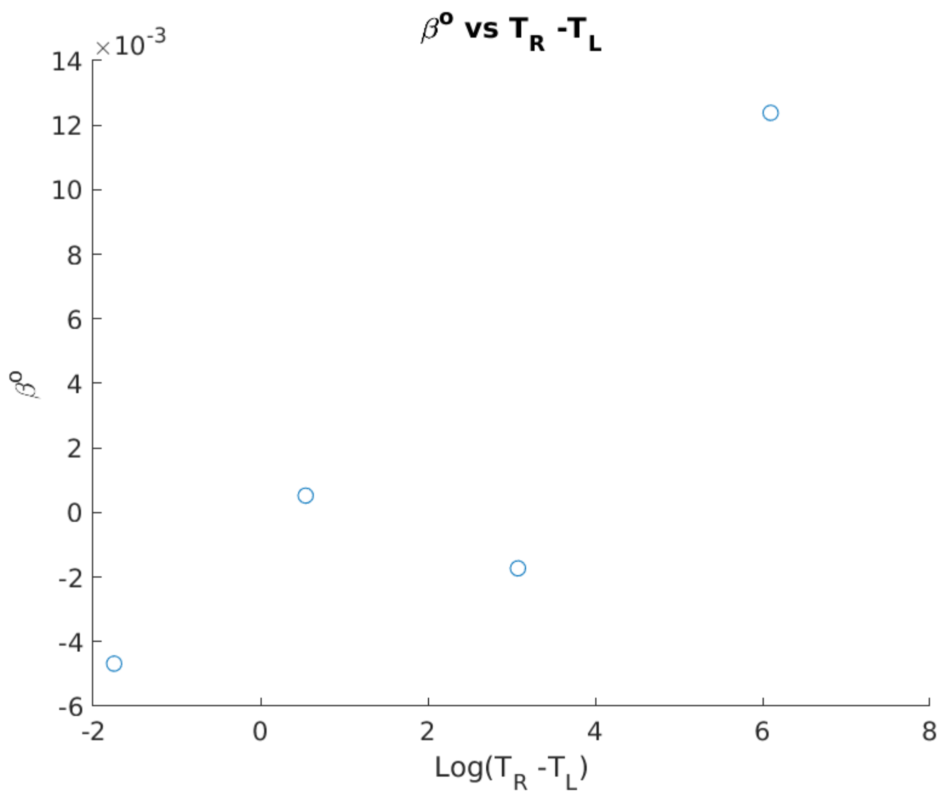


Figure 6.11: β^o vs $T_R - T_L$ - Stationary GLE: β^o does not appear to depend strongly on $T_R - T_L$.

6.4 Comparison to Other Thermostats

6.4.1 Langevin-Thermostats

The Langevin equations are SDEs with free or fixed boundary condition defined by:

$$d\dot{q}_1 = (\phi'(q_1 + q_2 + a) - \lambda \dot{q}_1)\, dt + \sqrt{2\lambda T_L} dW_t^L, \tag{6.70}$$
$$\dot{q}_j = -\phi'(q_j - q_{j-1} + a) + \phi'(q_{j+1} - q_j + a) \quad j = 2, \dots, N-1, \tag{6.71}$$
$$d\dot{q}_N = (-\phi'(q_{N-1} - q_N + a) - \lambda \dot{q}_N) + \sqrt{2\lambda T_R} dW_t^R, \tag{6.72}$$

for free boundary conditions, and

$$d\dot{q}_1 = (-\phi'(q_1 + a) + \phi'(q_1 + q_2 + a) - \lambda \dot{q}_1)\, dt + \sqrt{2\lambda T_L} dW_t^L, \tag{6.73}$$

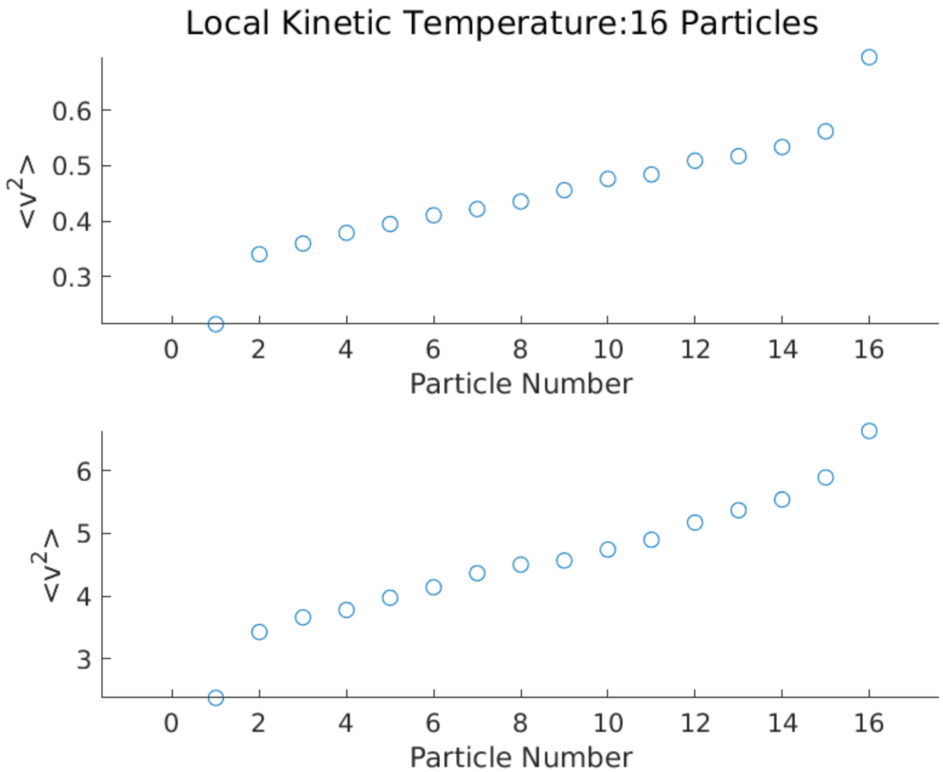
$$\ddot{q}_j = -\phi'(q_j - q_{j-1} + a) + \phi'(q_{j+1} - q_j + a) \quad j = 2, \ldots, N-1, \tag{6.74}$$

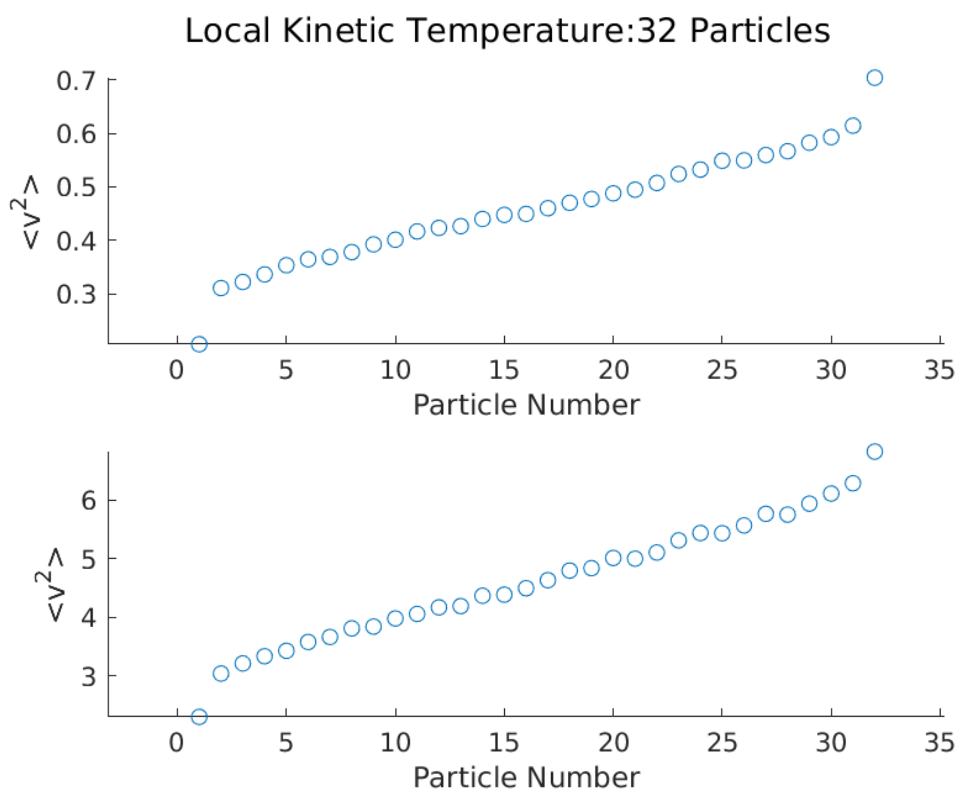
$$d\dot{q}_N = (\phi'(q_N + a) - \phi'(q_{N-1} - q_N + a) - \lambda \dot{q}_N)\, dt + \sqrt{2\lambda T_R} dW_t^R, \tag{6.75}$$

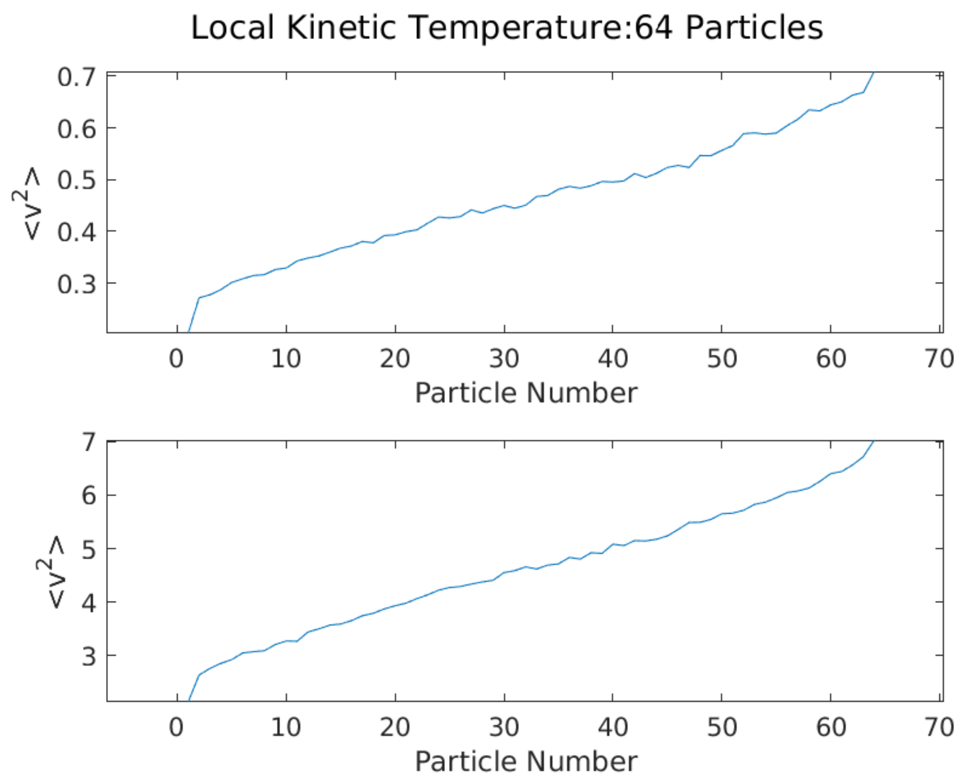
for the fixed boundary conditions, where W_t^L and W_t^R are independent Wiener processes. The friction parameter is $\lambda = 1$ for both baths. The interaction potential again is a confined Lennard-Jones potential. Because of the inclusion of the white noise term, the largest time scale of the solver is order $\sqrt{h}$, where h is the time step of the numerical scheme. In order to overcome numerical stiffness and have a large enough time step for long time numerical simulations, a velocity Verlet with an integrating factor method at the boundary points was the chosen numerical scheme. Systems of size 2^n, $n = 4, \ldots, 10$ were simulated. The final time of the simulations was 10,000, with time step $\Delta t = 0.001$. Sampling was performed beginning at time 5000 and samples of the position and velocities were recorded every one hundred steps. The bath temperatures for the simulations were $T_L = 0.2, T_R = 0.8$ and $T_L = 2, T_R = 8$ respectively. The initial conditions were random and chosen from the same distributions as the previous sections.

Free Boundary Condition

While the local kinetic temperature profile of bulk of the system remains fairly linear, the local kinetic temperature for small systems shows clear nonlinear behavior at the interfaces. For these smaller systems, while the left (colder) boundary particle has local temperature approximately the temperature of the left bath, the right (hotter) boundary particle does not reach its target temperature. As the system size increases this failure of the right boundary particle to have local kinetic temperature approximately the temperature of the bath is diminished. See figure 6.12 beginning on page 167.


Local Kinetic Temperature:16 Particles
$<v^2>$
Particle Number
$<v^2>$
Particle Number


Local Kinetic Temperature:32 Particles
$<v^2>$
Particle Number
$<v^2>$
Particle Number


Local Kinetic Temperature:64 Particles
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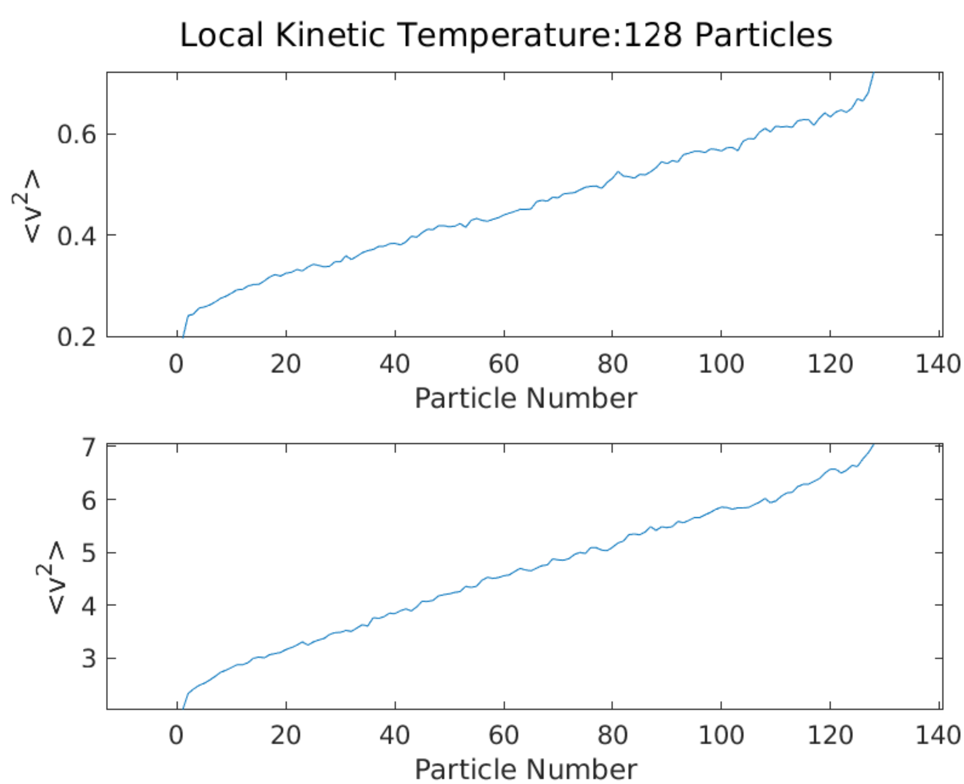
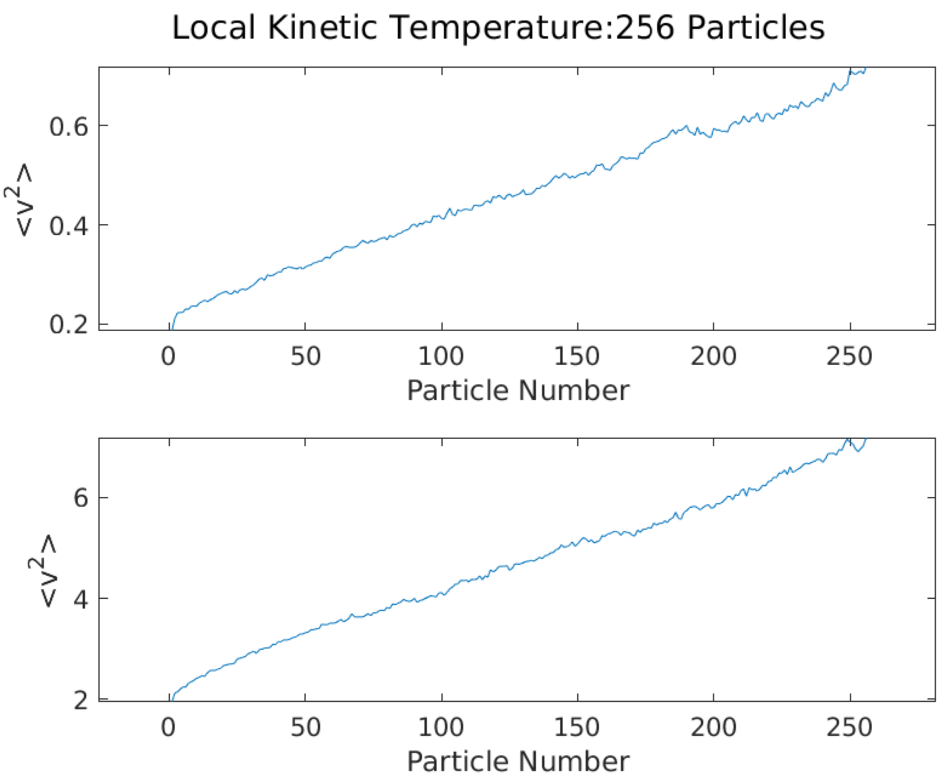
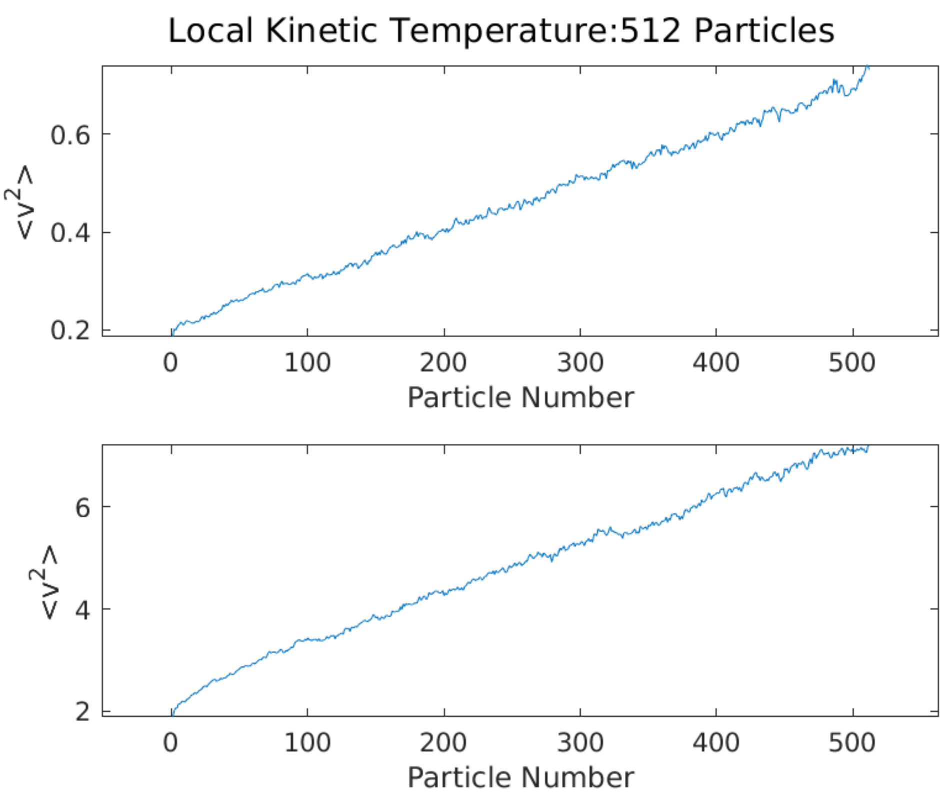
Particle Number
<v^2>
Particle Number


Local Kinetic Temperature:128 Particles
<v^2>
Particle Number
<v^2>
Particle Number



Local Kinetic Temperature:256 Particles
<v^2>
0.2
0.4
0.6
0
50
100
150
200
250
Particle Number
<v^2>
2
4
6
0
50
100
150
200
250
Particle Number



Local Kinetic Temperature:512 Particles
<v^2>
0.2
0.4
0.6
0
100
200
300
400
500
Particle Number
<v^2>
2
4
6
0
100
200
300
400
500
Particle Number

T_L - T_R	α	α°	$\alpha^\circ - \alpha$
0.2 - 0.8	1.3959	1.3955	-4×10^{-4}
2 - 8	1.3428	1.3421	-7×10^{-4}

Table 6.3: Langevin Equation Free Boundary Condition: Conductivity Scalings α and α^o

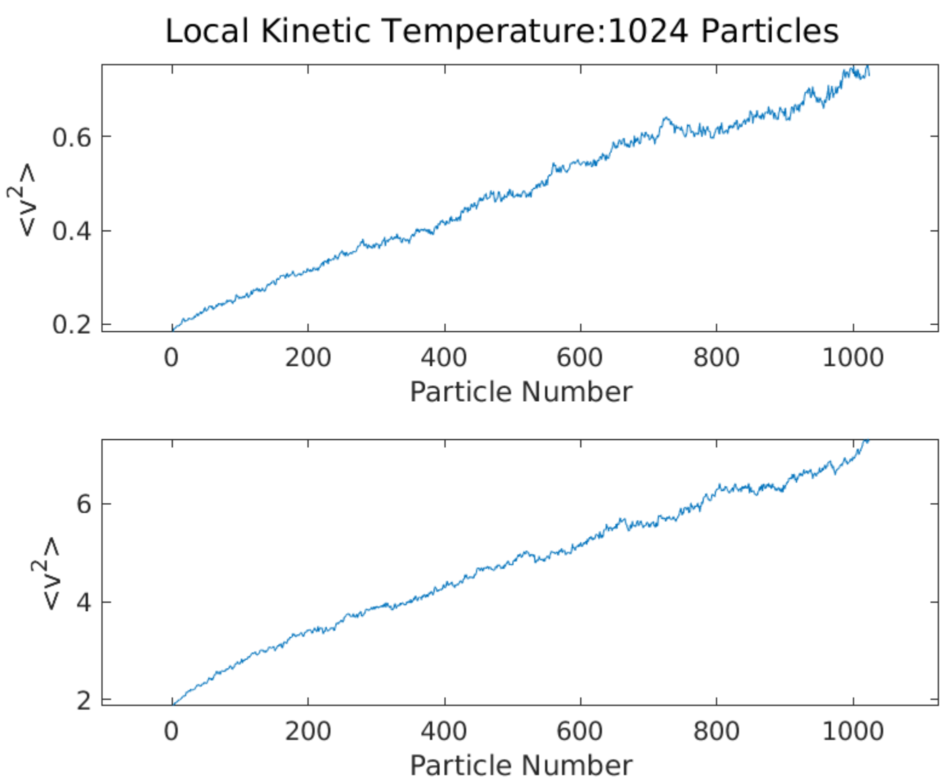
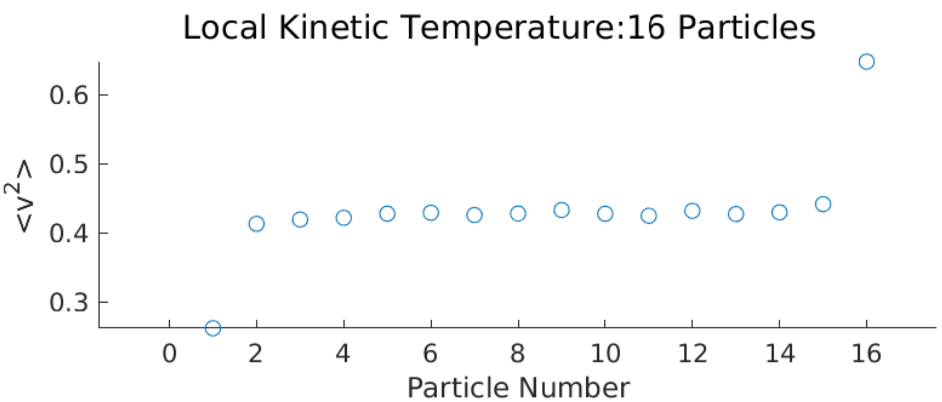


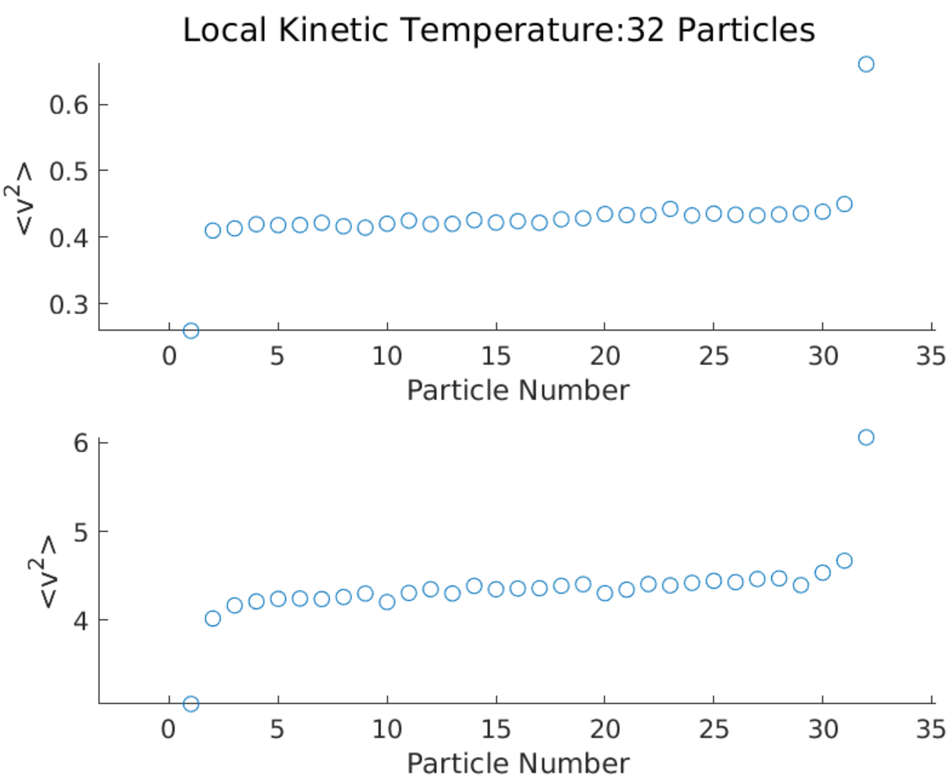
Figure 6.12: Local Kinetic Temperature - Langevin Thermostat with free boundary condition.

The linearity of the log-log plots of conductivity versus system size in figure 6.13 beginning on page 187 verify the validity of the scaling laws $\kappa \propto N^\alpha$ and $\kappa^o \propto N^{\alpha^o}$. The limit of small oscillations seems to hold for this thermostat and selected parameters: when the left and right baths temperatures are $T_L = 0.2, T_R = 0.8$ we have $\alpha = 1.3959$ and $\alpha^o = 1.3955$ and when $T_L = 2, T_R = 8$ we have $\alpha = 1.3428$ and $\alpha^o = 1.3421$. These values are also shown in table 6.3 on page 167. The positivity of α and α^o indicates that heat flow does not obey Fourier's law.

Fixed Boundary Condition

The Langevin thermostat with fixed boundary conditions has discontinuities and/or non-linearities in the local kinetic temperature profile that are visible at all investigated system sizes and temperatures. For all investigated systems, both the left and right boundary particles failed to reach their target local kinetic temperatures. Moreover, because of the large discontinuities in the local kinetic temperature present, while the local kinetic temperature of the interior particles is linear, the slope is far smaller than Fourier's law would predict. See figure 6.14 beginning on page 172.


Local Kinetic Temperature:16 Particles
$<v^2>$
0.6
0.5
0.4
0.3
0
2
4
6
8
10
12
14
16
Particle Number
$<v^2>$
6
5
4
0
2
4
6
8
10
12
14
16
Particle Number


Local Kinetic Temperature:32 Particles
$<v^2>$
0.6
0.5
0.4
0.3
0
5
10
15
20
25
30
35
Particle Number
$<v^2>$
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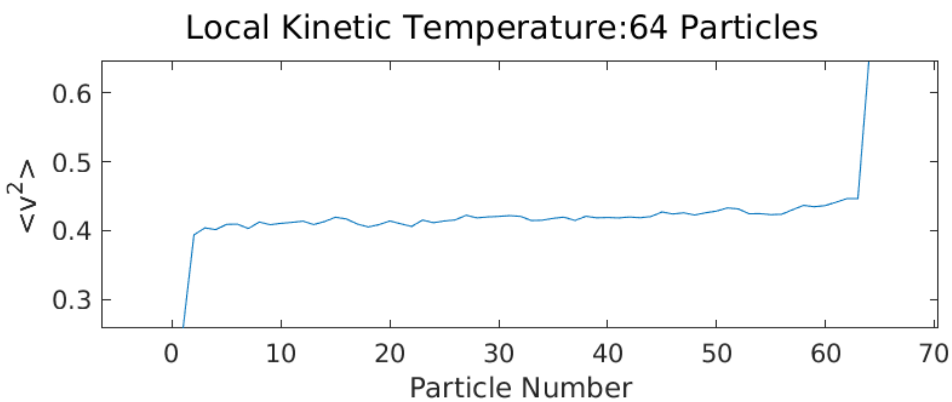
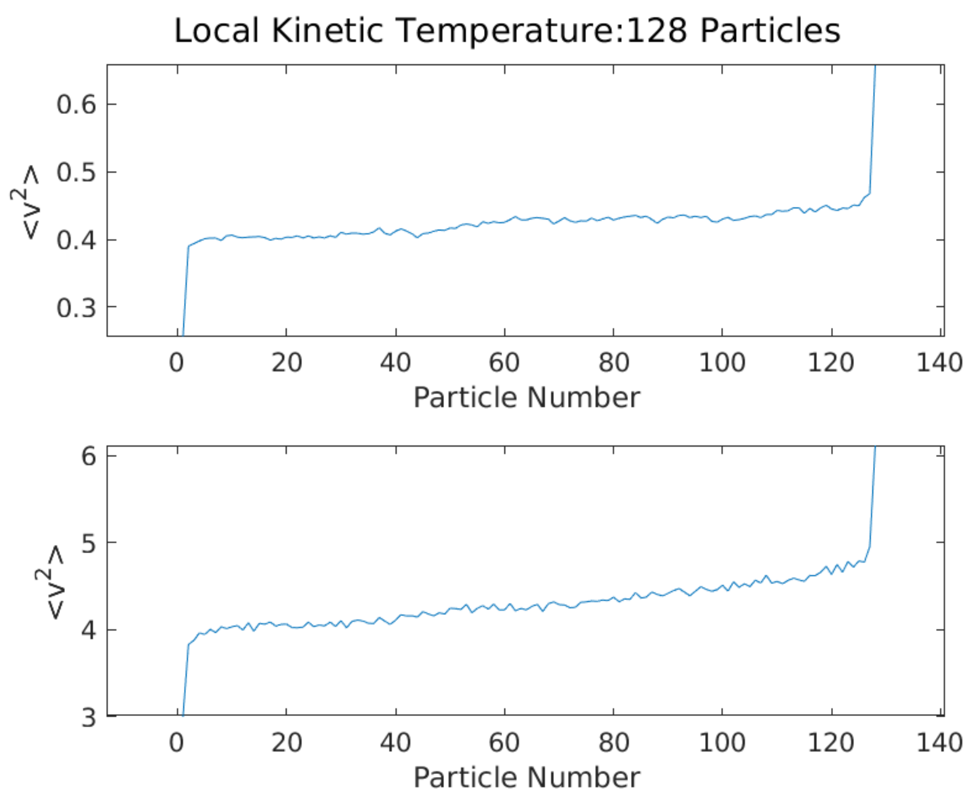
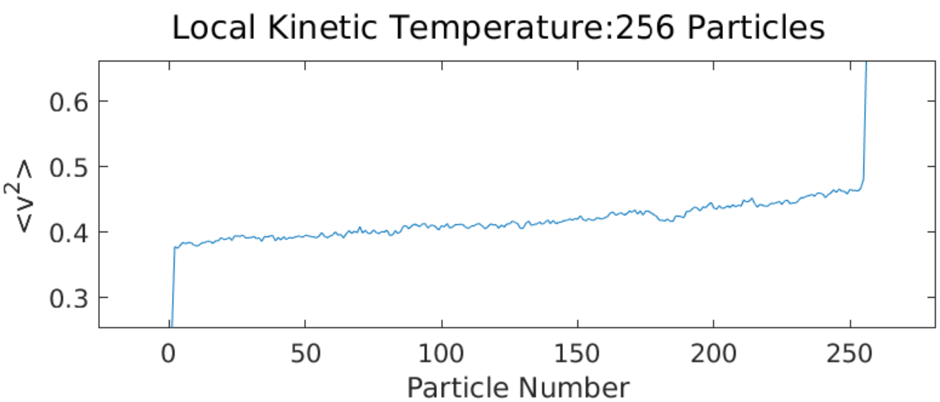
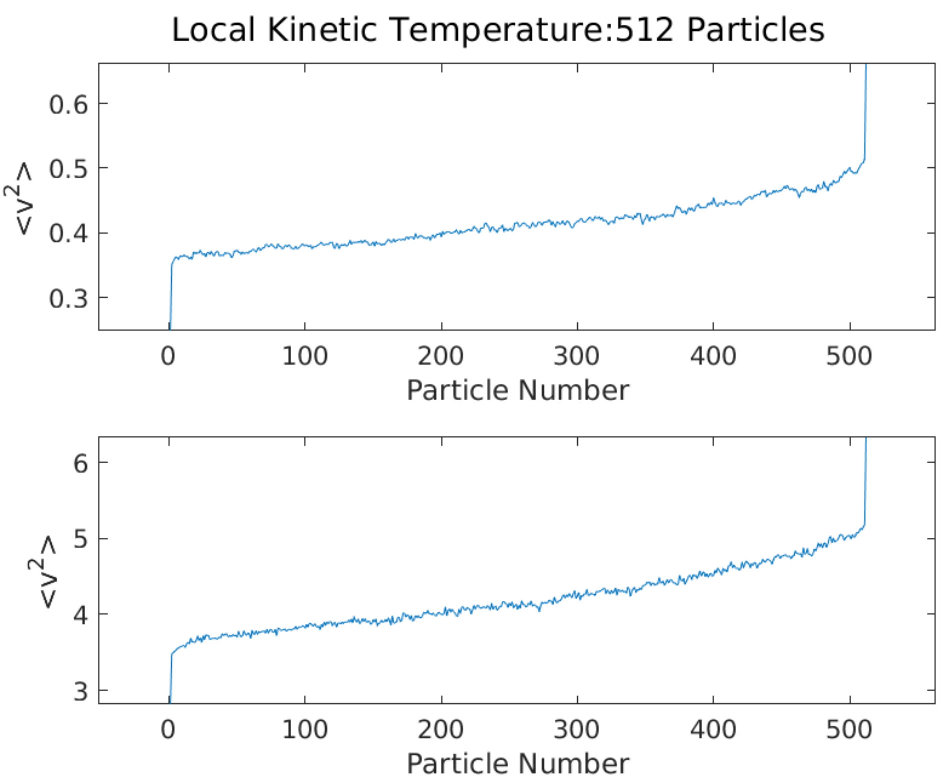
5
4
0
5
10
15
20
25
30
35
Particle Number


Local Kinetic Temperature:64 Particles
<v2>
0.6
0.5
0.4
0.3
0
10
20
30
40
50
60
70
Particle Number
<v2>
6
5
4
0
10
20
30
40
50
60
70
Particle Number


Local Kinetic Temperature:128 Particles
<v2>
0.6
0.5
0.4
0.3
0
20
40
60
80
100
120
140
Particle Number
<v2>
6
5
4
3
0
20
40
60
80
100
120
140
Particle Number


Local Kinetic Temperature:256 Particles
<v^2>
0.6
0.5
0.4
0.3
0
50
100
150
200
250
Particle Number
<v^2>
6
5
4
3
0
50
100
150
200
250
Particle Number


Local Kinetic Temperature:512 Particles
<v^2>
0.6
0.5
0.4
0.3
0
100
200
300
400
500
Particle Number
<v^2>
6
5
4
3
0
100
200
300
400
500
Particle Number

T_L - T_R	α	α°	$\alpha^\circ - \alpha$
0.2 - 0.8	1.9274	1.9272	-2×10^{-4}
2 - 8	1.889	1.8883	-7×10^{-4}

Table 6.4: Langevin Equation Fixed Boundary: Conductivity Scalings α and α^o

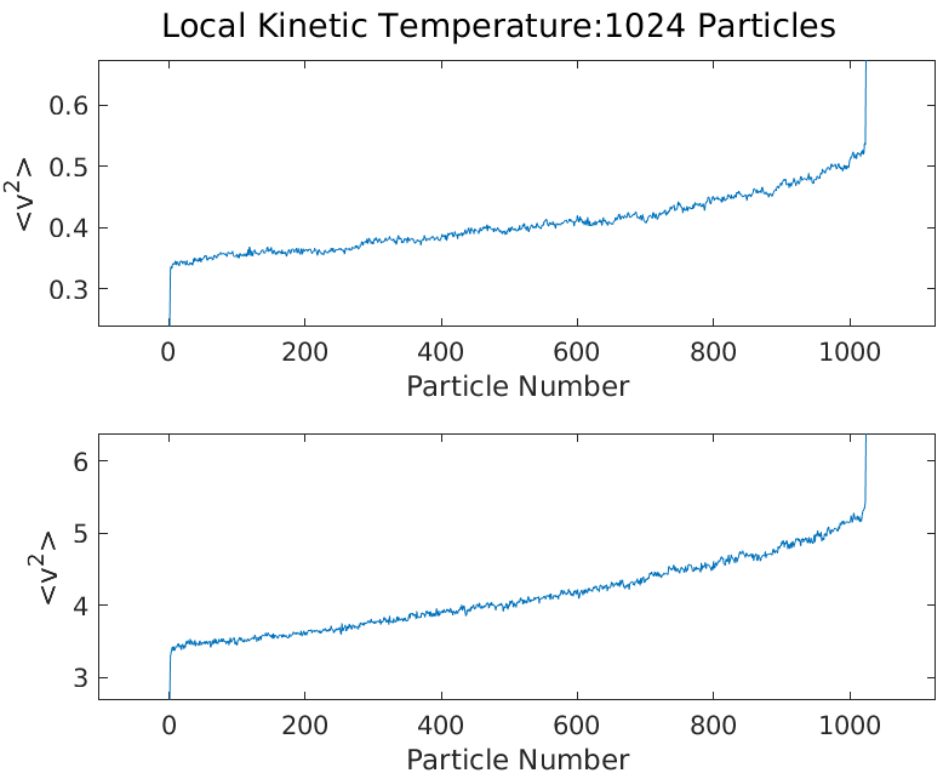


Figure 6.14: Local Kinetic Temperature: Langevin Thermostat with fixed boundary condition.

Plotting the conductivities versus the system size in log scale (figure 6.15 on page 187) shows the validity of the scaling of κ and κ^o as N^α and N^{α^o} respectively. Similar to the free case, the limit of small oscillations hold for the Langevin thermostat for the selected parameters. When the left and right baths temperatures are $T_L = 0.2, T_R = 0.8$ we have $\alpha = 1.9274$ and $\alpha^o = 1.9272$ and when $T_L = 2, T_R = 8$ we have $\alpha = 1.889$ and $\alpha^o = 1.8883$. These values are also shown in table 6.4 on page 172.

6.4.2 Nosé-Hoover Thermostat

We consider a system of particles interacting with nearest neighbor confined Lennard-Jones potentials ϕ with free and fixed boundary conditions attached to two Nosé-Hoover thermostats. To maintain consistency with the other sections only the boundary particles are allowed to interact with the baths. This leads to the equations of motion for the free system

$$\ddot{q}_1 = \phi'(q_1 + q_2 + a) - \eta_L \dot{q}_1, \tag{6.76}$$
$$\ddot{q}_j = -\phi'(q_j - q_{j-1} + a) + \phi'(q_{j+1} - q_j + a) \quad j = 2, \ldots, N-1, \tag{6.77}$$
$$\ddot{q}_N = -\phi'(q_{N-1} - q_N + a) + \eta_R \dot{q}_N, \tag{6.78}$$
$$\dot{\eta}_L = \frac{1}{\Theta_L^2}\left(\frac{\dot{q}_1^2}{T_L} - 1\right), \tag{6.79}$$
$$\dot{\eta}_R = \frac{1}{\Theta_R^2}\left(\frac{\dot{q}_N^2}{T_R} - 1\right), \tag{6.80}$$

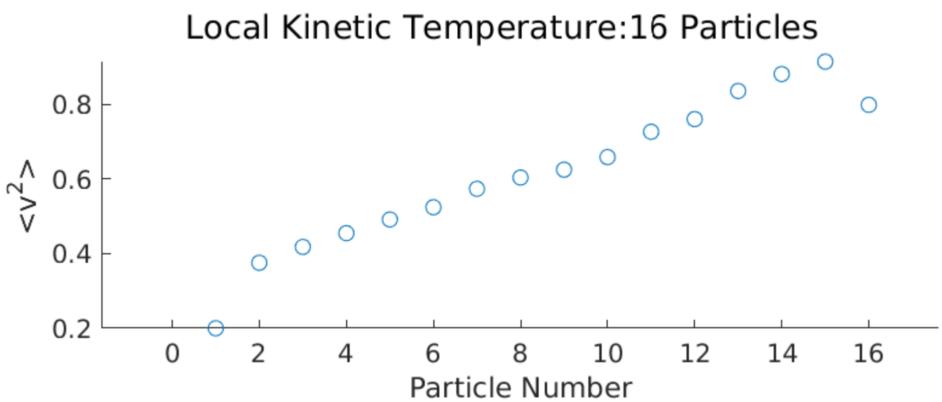
and for the fixed system

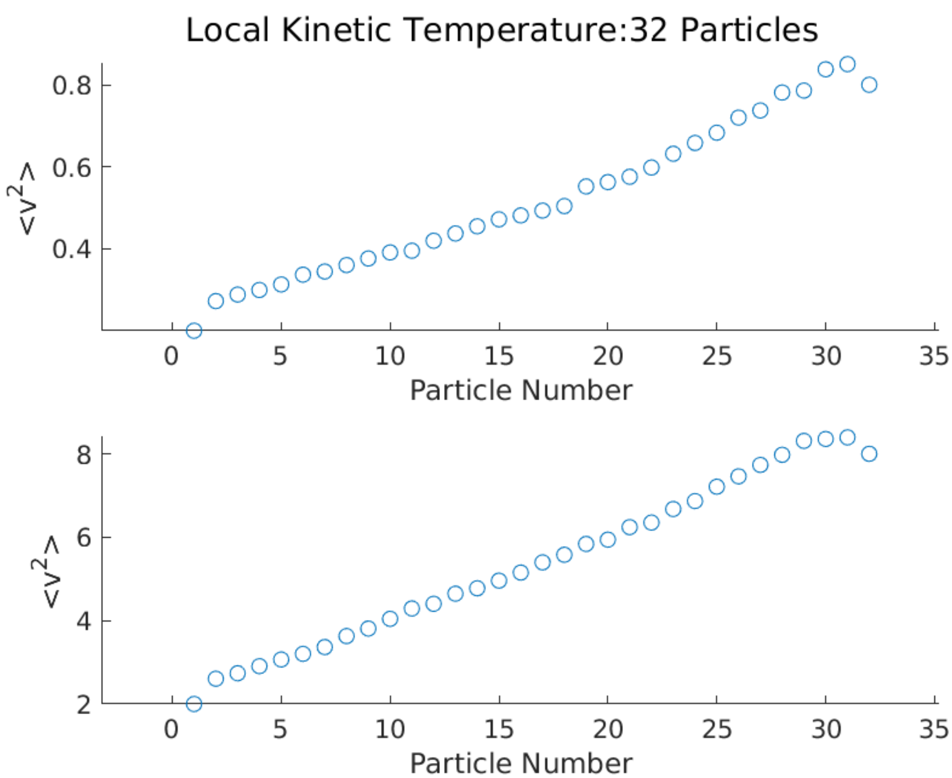
$$\ddot{q}_1 = -\phi'(q_1 + a) + \phi'(q_1 + q_2 + a) - \eta_L \dot{q}_1, \tag{6.81}$$
$$\ddot{q}_j = -\phi'(q_j - q_{j-1} + a) + \phi'(q_{j+1} - q_j + a), \quad j = 2, \ldots, N-1, \tag{6.82}$$
$$\ddot{q}_N = \phi'(q_N + a) - \phi'(q_{N-1} - q_N + a) + \eta_R \dot{q}_N, \tag{6.83}$$
$$\dot{\eta}_L = \frac{1}{\Theta_L^2}\left(\frac{\dot{q}_1^2}{T_L} - 1\right), \tag{6.84}$$
$$\dot{\eta}_R = \frac{1}{\Theta_R^2}\left(\frac{\dot{q}_N^2}{T_R} - 1\right). \tag{6.85}$$

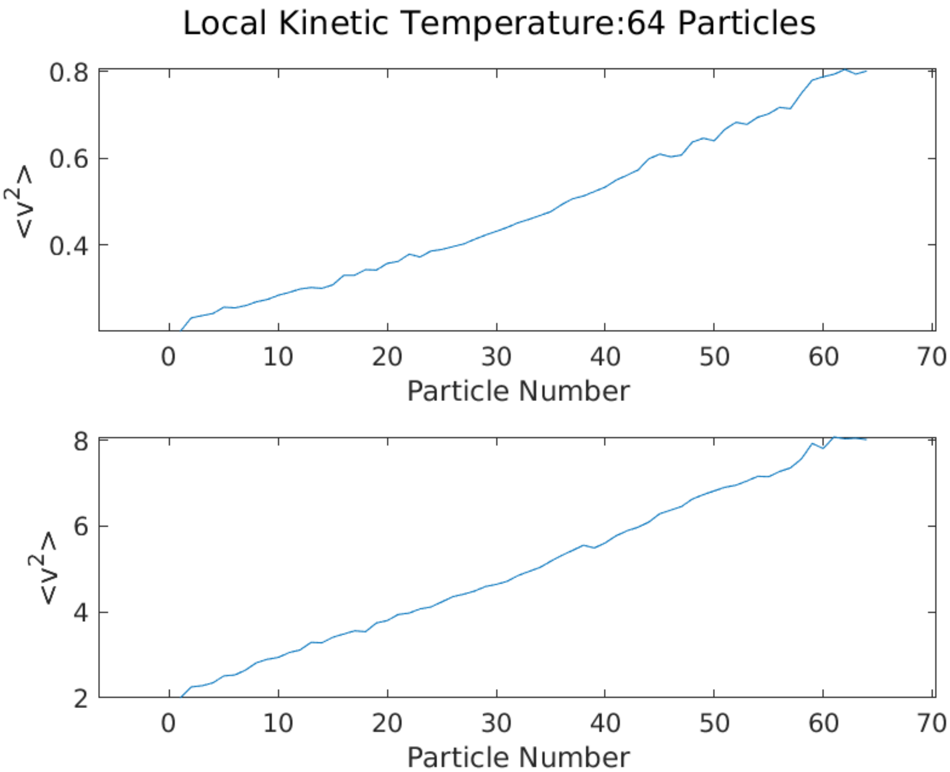
Systems of size 2^N, $N = 4, \ldots, 10$ were simulated using RK3. In all the experiments, the Nosé-Hoover coupling parameter $\Theta = 1$ for both baths. The initial conditions were random with the same distributions as the previous sections. The final time of the simulation is again $10,000$ and the time step is $\Delta t = 0.001$. Sampling begins at time 5000 and samples of the position and velocity are taken every one hundred steps.

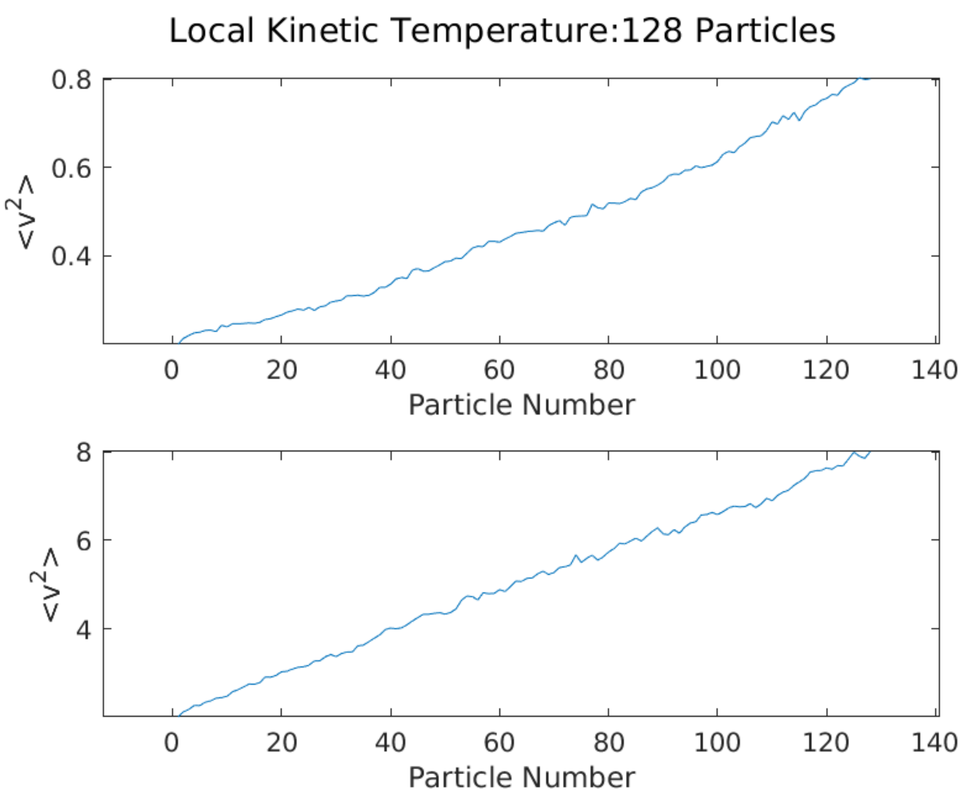
Free Boundary Condition

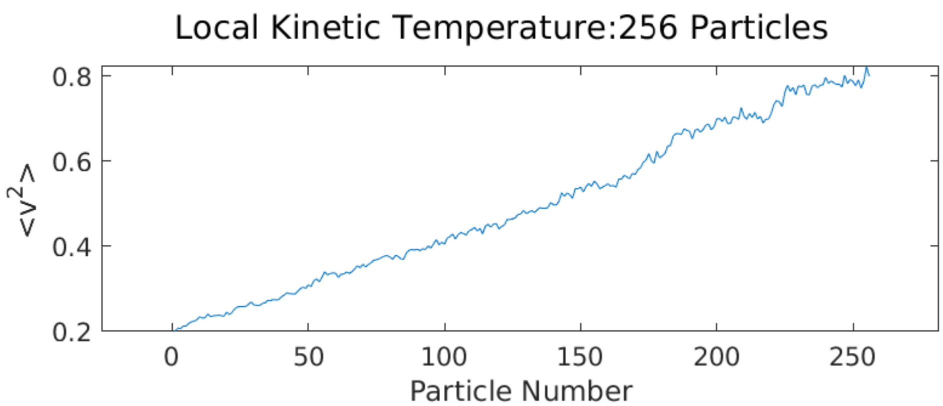
The local temperature profiles when using the free boundary condition is shown in figure 6.16 beginning on page 178. Systems with 16 and 32 particles both exhibit a dip in the temperatures at the boundaries.

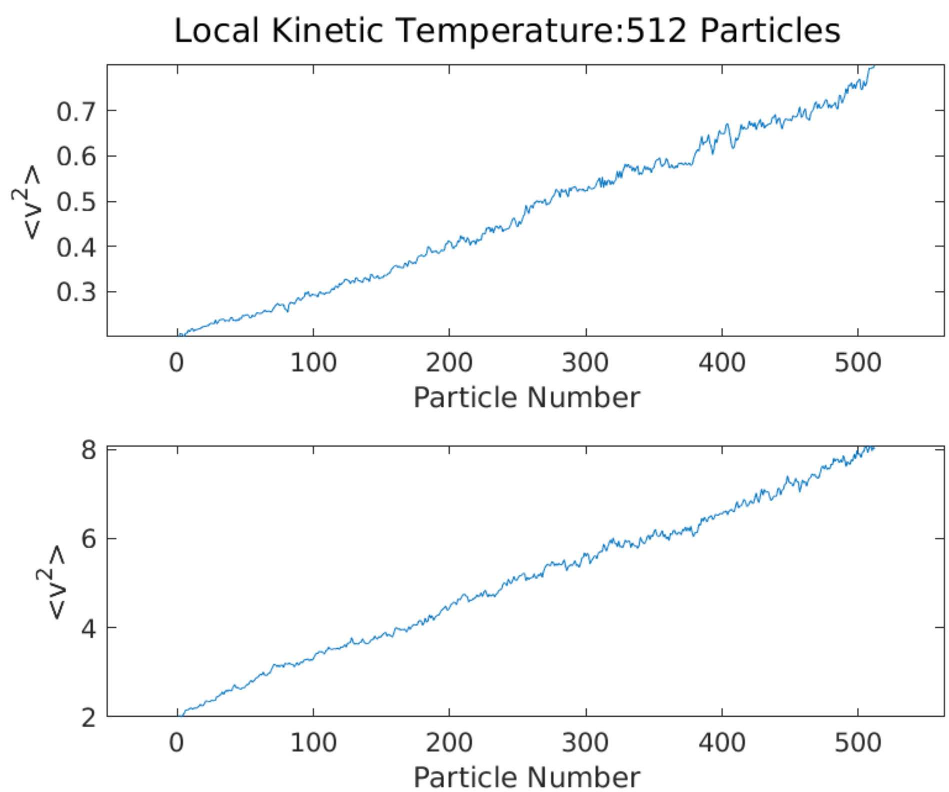

Local Kinetic Temperature:16 Particles
$<v^2>$
0.2
0.4
0.6
0.8
0 2 4 6 8 10 12 14 16
Particle Number
$<v^2>$
4
6
8
0 2 4 6 8 10 12 14 16
Particle Number


Local Kinetic Temperature:32 Particles
$<v^2>$
0.4
0.6
0.8
0 5 10 15 20 25 30 35
Particle Number
$<v^2>$
2
4
6
8
0 5 10 15 20 25 30 35
Particle Number


Local Kinetic Temperature:64 Particles
<v^2>
0.8
0.6
0.4
0
10
20
30
40
50
60
70
Particle Number
<v^2>
8
6
4
2
0
10
20
30
40
50
60
70
Particle Number


Local Kinetic Temperature:128 Particles
<v^2>
0.8
0.6
0.4
0
20
40
60
80
100
120
140
Particle Number
<v^2>
8
6
4
0
20
40
60
80
100
120
140
Particle Number


Local Kinetic Temperature:256 Particles
<v2>
0.8
0.6
0.4
0.2
0
50
100
150
200
250
Particle Number
8
6
4
Particle Number


Local Kinetic Temperature:512 Particles
<v2>
0.7
0.6
0.5
0.4
0.3
0
100
200
300
400
500
Particle Number
8
6
4
2
Particle Number

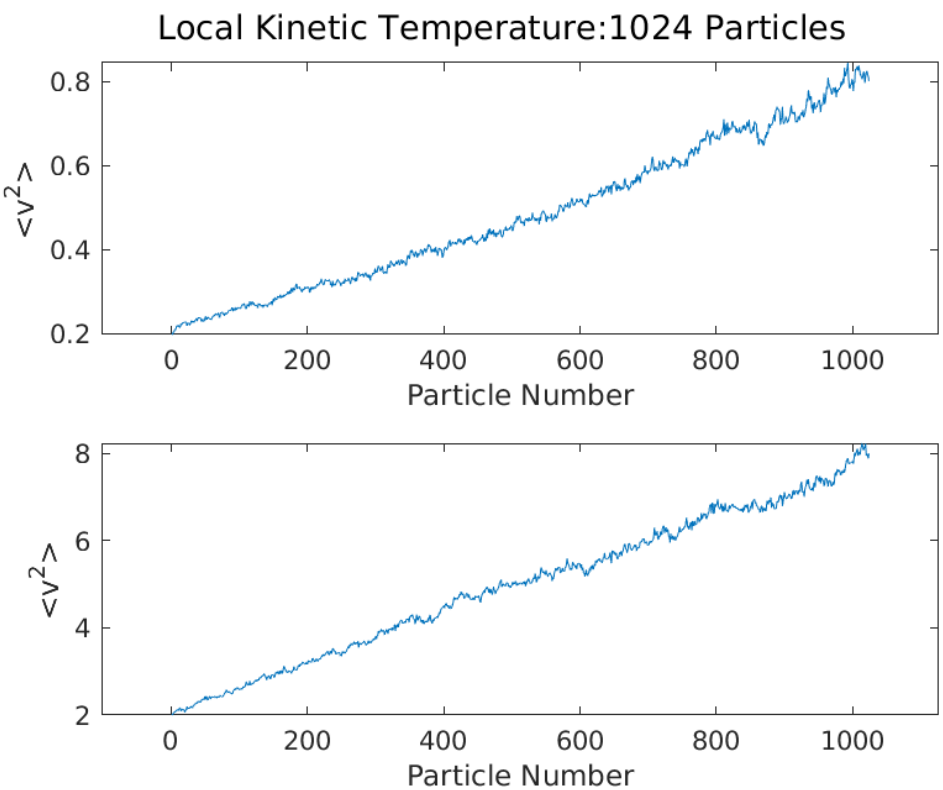


Figure 6.16: Local Kinetic Temperature - Nosé-Hoover Free Boundary: The Nosé-Hoover thermostats exhibit linear behavior throughout except at the boundaries of small systems.

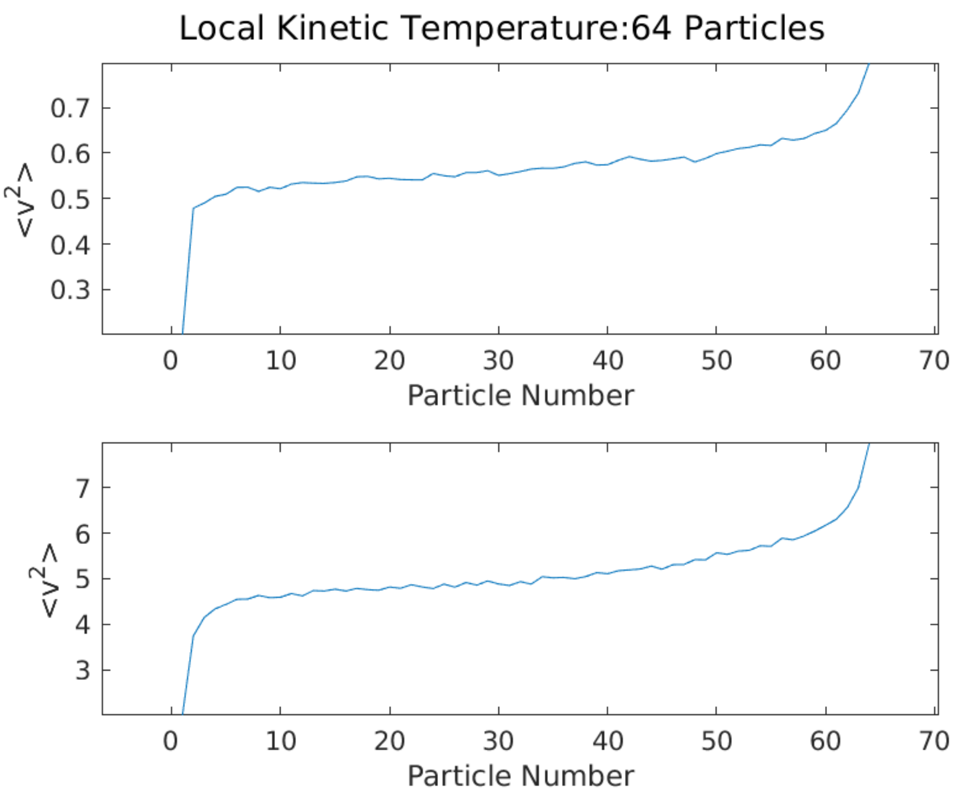
Calculating α and α^o and the log-log plots of conductivity versus system size reveals some more interesting behavior of the Nosé-Hoover thermostat. As seen in 6.17 beginning on page 188 the colder simulation exhibits a linear scaling in the log-log plot indicating that the conductivity scales proportionally to N^α. However for the warmer system, there is fairly substantial deviation of the data points from the linear best fit. This indicates that conductivity for warmers systems does not truly scale as N^α, but has a more complicated dependence. When one calculates the conductivity in the limit of small oscillations, one sees a linear dependence in the log-log plots of κ^o vs N. This indicates that the conductivity in the limit of small oscillations is proportional to N^{α^o}. Interestingly though, for the colder bath, α^o and α are substantially different, while for the warmer bath they are not (see table 6.5 on page 179). The positivity of α and α^o however indicate the anomalous behavior of the heat flow and the failure of Fourier's law.

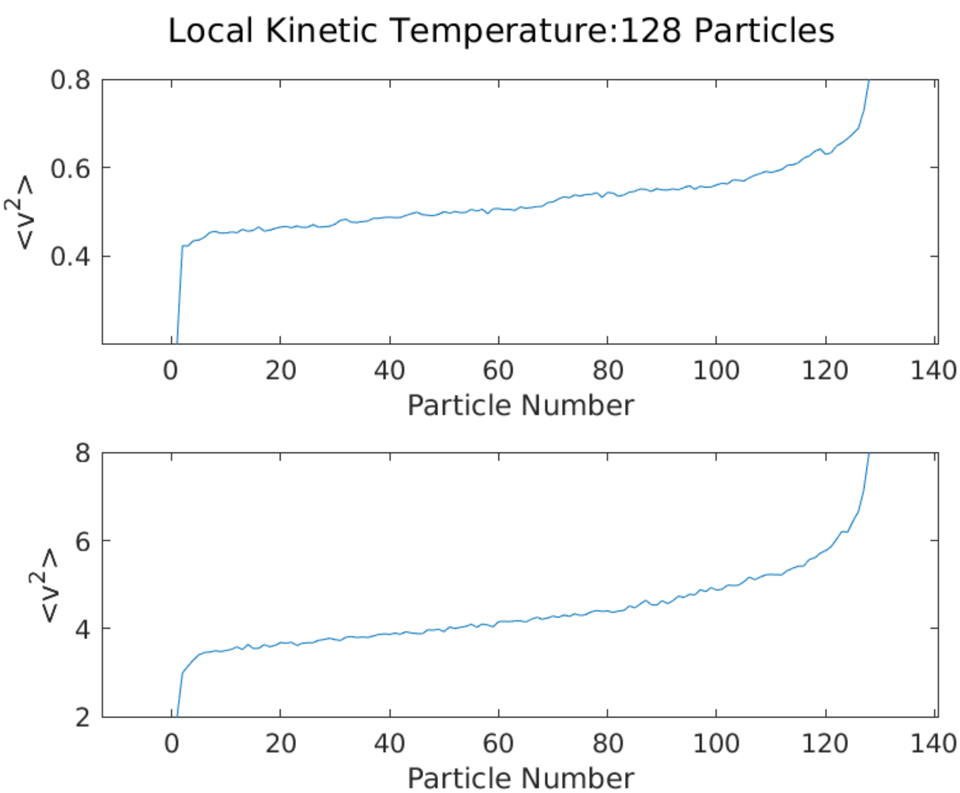
T_L - T_R	α	α°	$\alpha^\circ - \alpha$
0.2 - 0.8	1.2687	0.89197	-0.37673
2 - 8	1.3052	1.2604	-0.0448

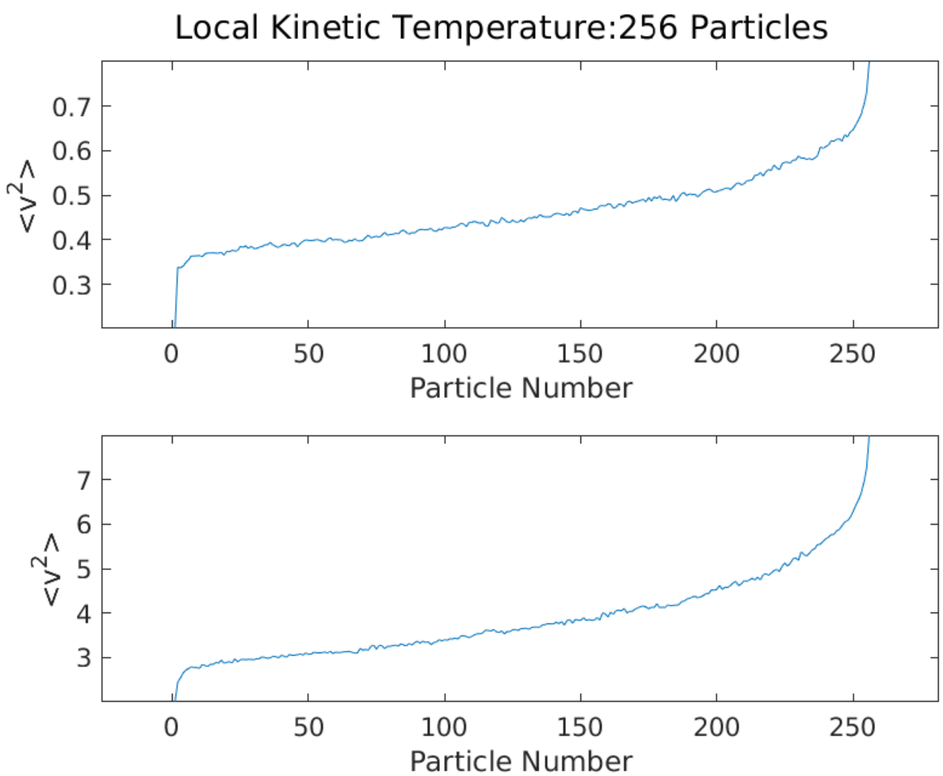
Table 6.5: Nosé Hoover thermostat with free boundary condition: Conductivity Scalings α and α^o

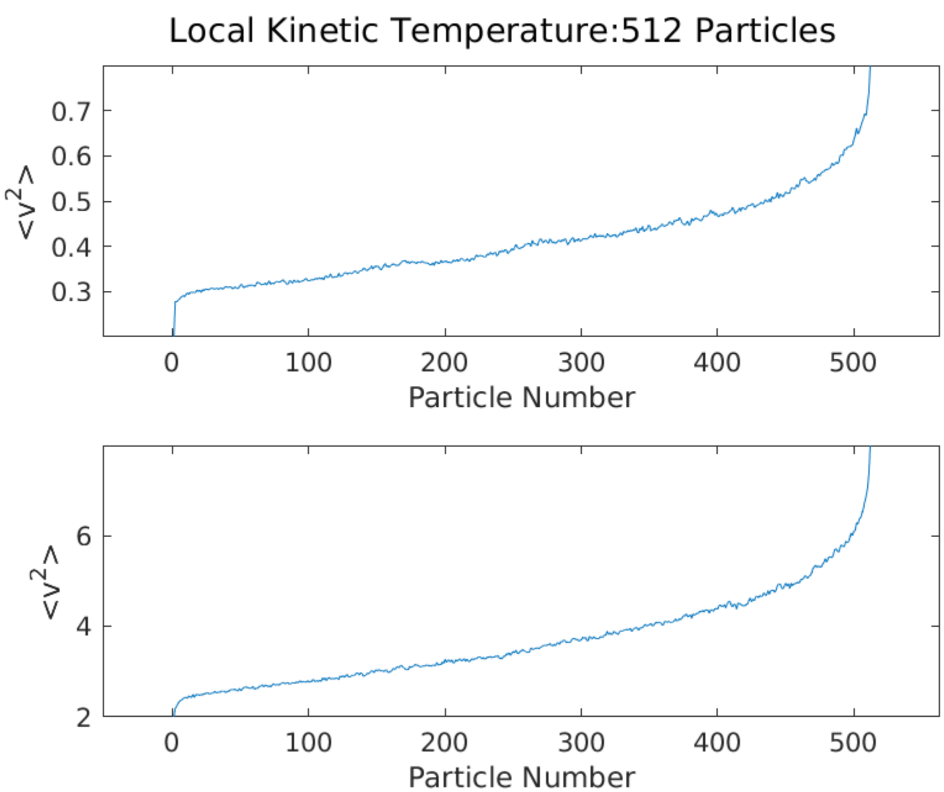
Fixed Boundary Condition

When fixed boundary conditions are used the behavior of the local temperature profile changes significantly. All system scales exhibit clear non-linear behavior at both interfaces. At the left (colder) bath, the local kinetic temperature seems to have a discontinuity for all system sizes. The size of the discontinuity decreases as the system size increases, but remains even for the system with 1024 particles. The right (hotter) interface does not exhibit the same discontinuity, but an exponential increase until to the right bath temperature. The Nosé-Hoover thermostat successfully keeps the boundary particles at the selected temperatures. See figure 6.18 beginning on page 182.


Local Kinetic Temperature:64 Particles
$<v^2>$
0.7
0.6
0.5
0.4
0.3
0
10
20
30
40
50
60
70
Particle Number
$<v^2>$
7
6
5
4
3
0
10
20
30
40
50
60
70
Particle Number


Local Kinetic Temperature:128 Particles
$<v^2>$
0.8
0.6
0.4
0
20
40
60
80
100
120
140
Particle Number
$<v^2>$
8
6
4
2
0
20
40
60
80
100
120
140
Particle Number


Local Kinetic Temperature:256 Particles
$<v^2>$
0.7
0.6
0.5
0.4
0.3
0
50
100
150
200
250
Particle Number
$<v^2>$
7
6
5
4
3
0
50
100
150
200
250
Particle Number


Local Kinetic Temperature:512 Particles
$<v^2>$
0.7
0.6
0.5
0.4
0.3
0
100
200
300
400
500
Particle Number
$<v^2>$
6
4
2
0
100
200
300
400
500
Particle Number

T_L - T_R	α	α°	$\alpha^\circ - \alpha$
0.2 - 0.8	1.7742	1.7729	-1.3×10^{-3}
2 - 8	1.6348	1.6338	-1×10^{-3}

Table 6.6: Nosé Hoover thermostat with free boundary condition: Conductivity Scalings α and α^o

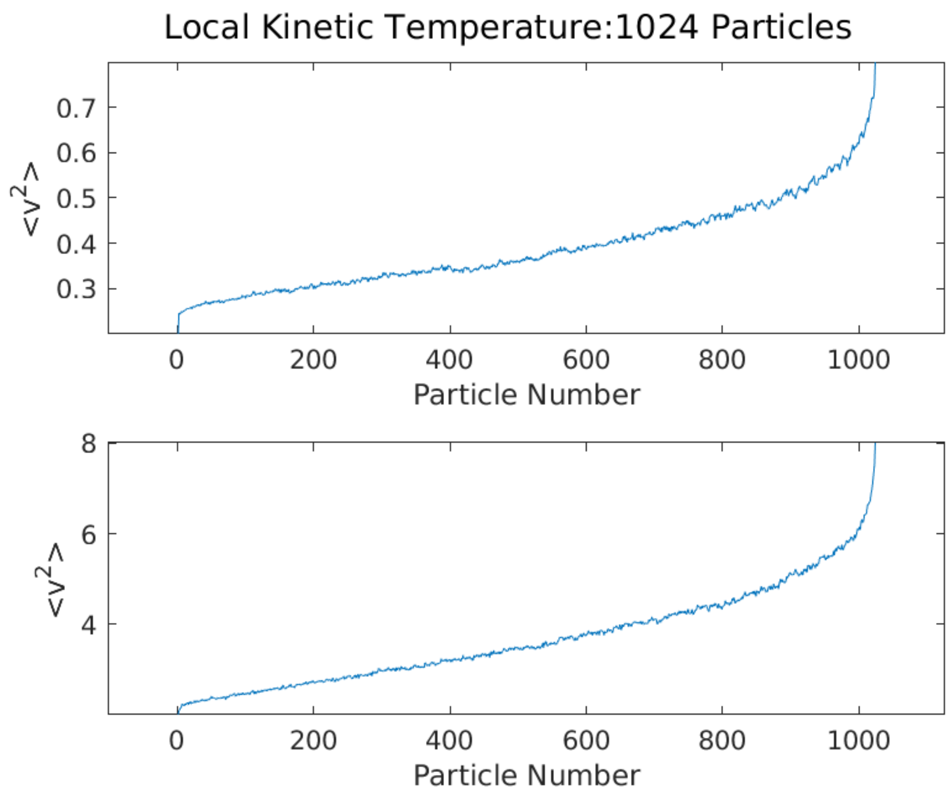


Figure 6.18: Local Kinetic Temperature: The Nosé-Hoover thermostats exhibit linear behavior throughout except at the boundaries of small systems.

The linearity of the log-log plots of conductivity vs. system size in figure 6.19 beginning on page 190 confirms that the conductivities scale as N^α and N^{α^o}. Moreover, the scaling coefficients α and α^o are nearly identical with differences on the order of 10^{-3}. See table 6.6 on page 182. The positivity of α and α^o indicates that heat flow does not obey Fourier's law.

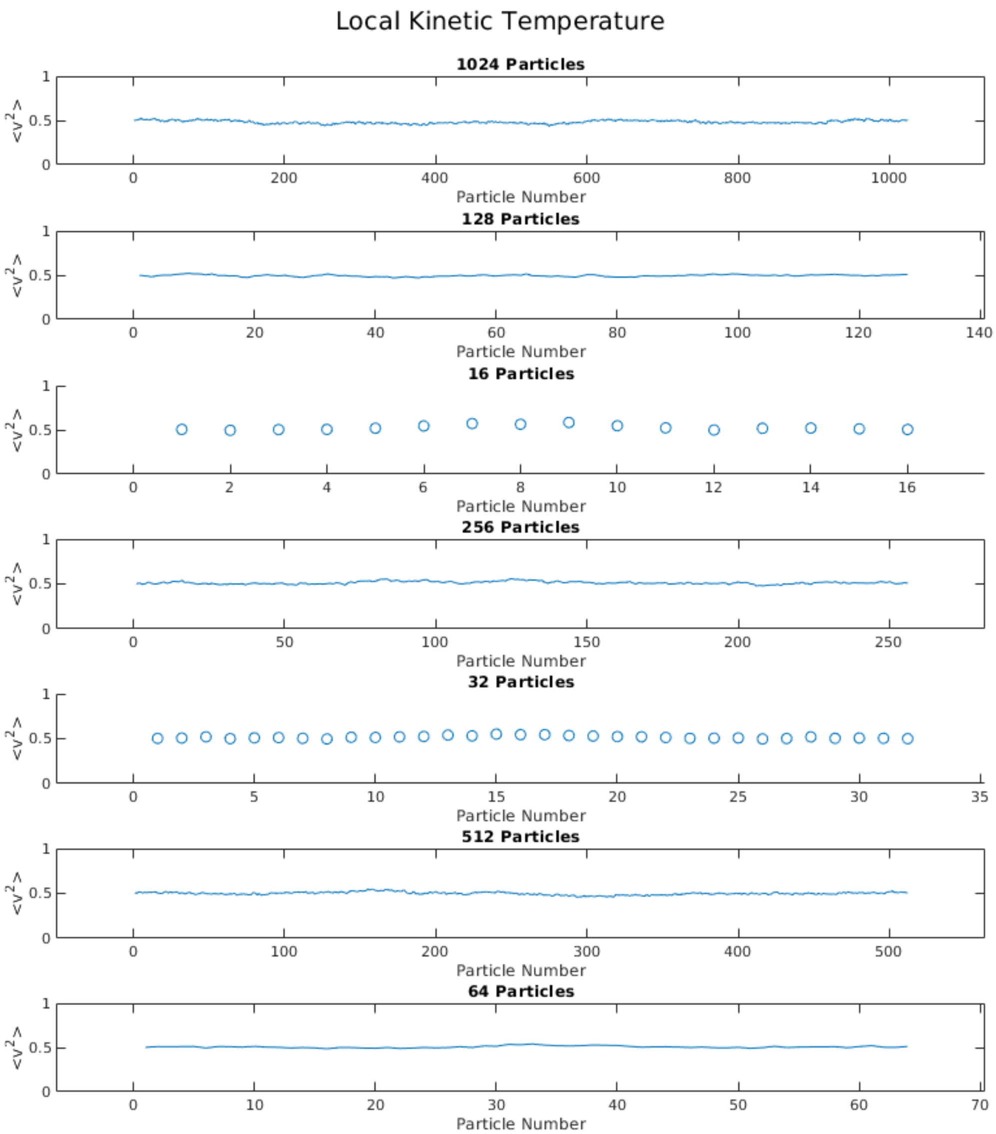


Figure 6.1: Local Kinetic Temperature - Non-Stationary GLE: The flat temperature profile of all systems indicated the system equilibriated.

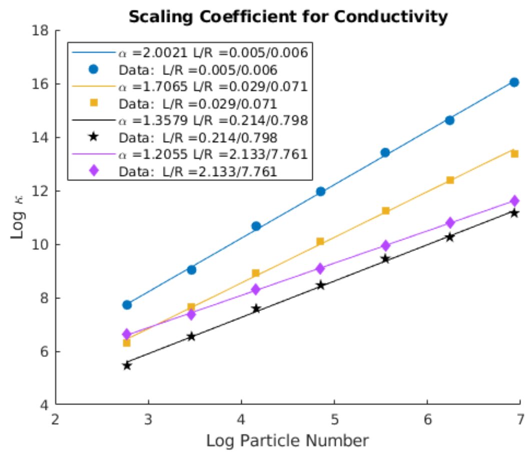


Figure 6.3: Log κ vs $\log(N)$ - Non-Stationary GLE: Linear profiles indicate validity scaling κ as N^{α}.

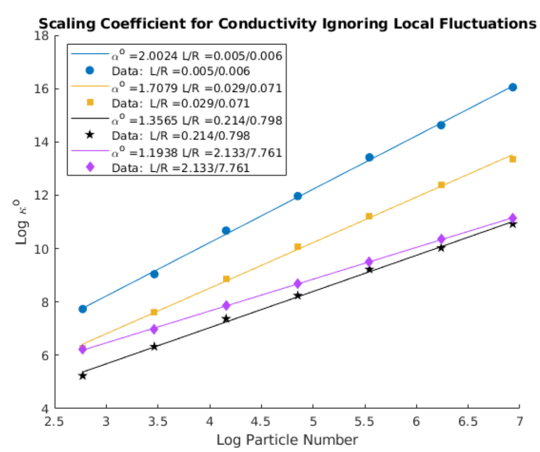


Figure 6.4: Log κ^o vs $\log(N)$ - Non-Stationary GLE: Linear profiles indicate validity scaling κ^o as N^{α^o}.

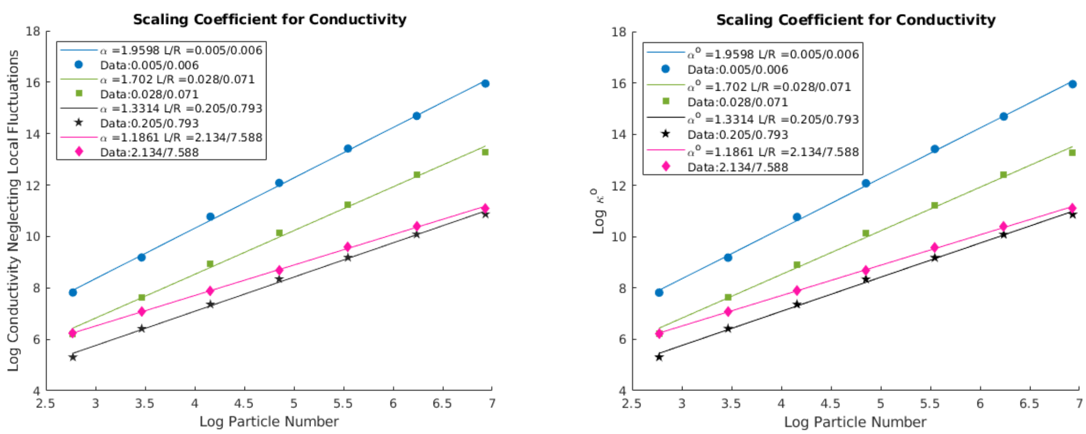
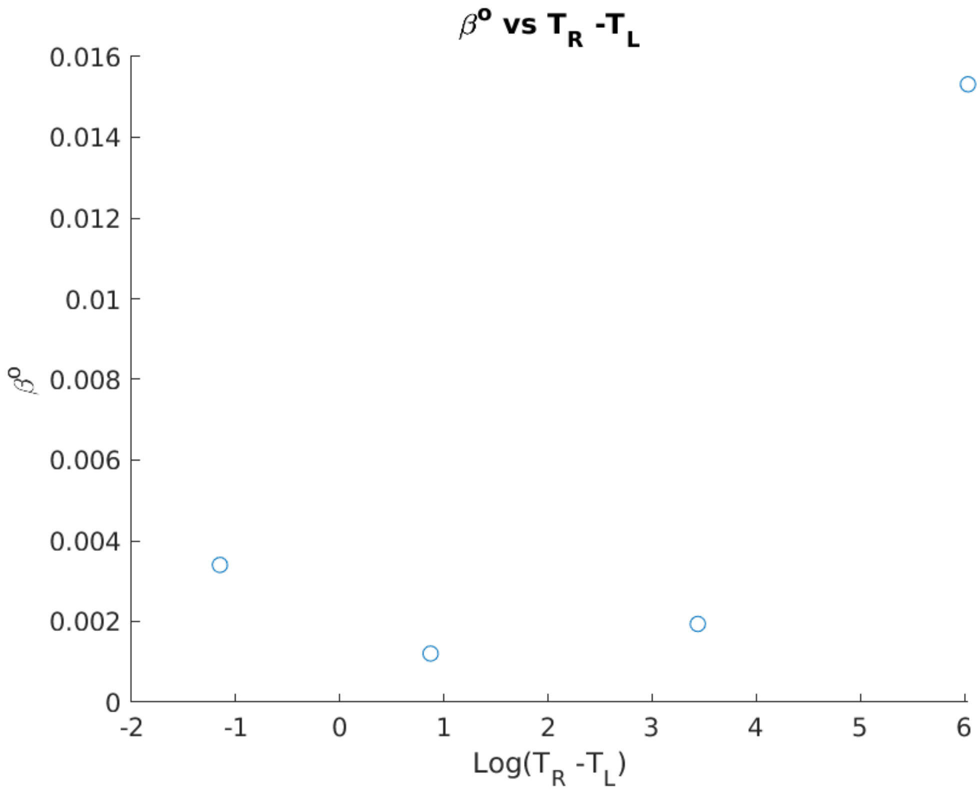
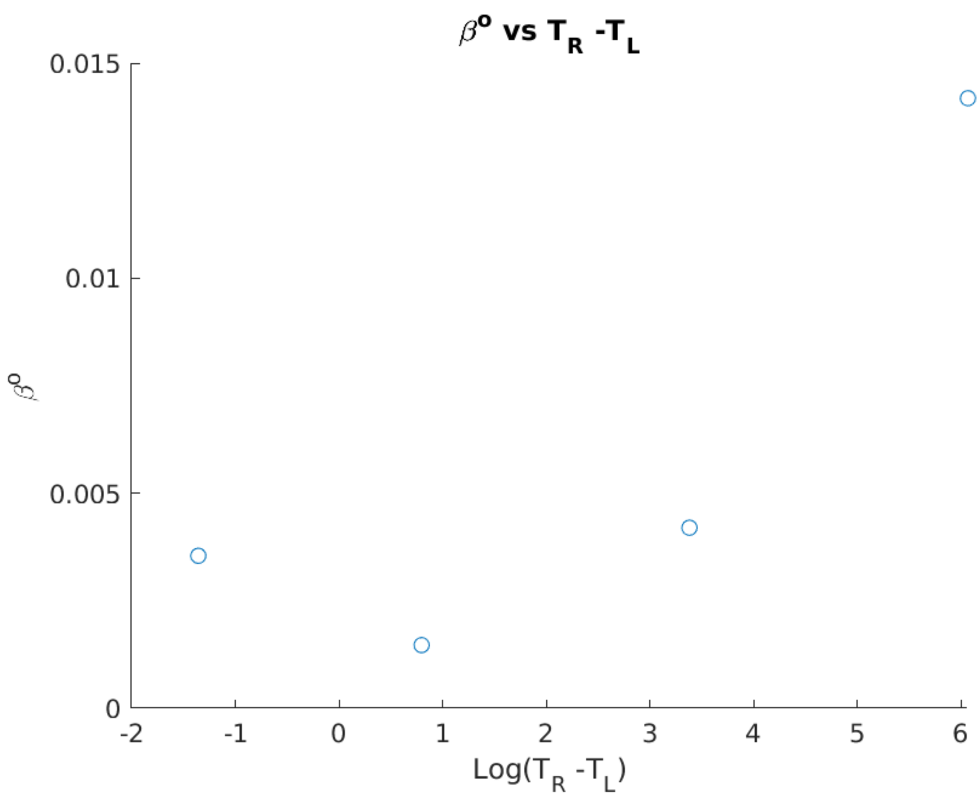


Figure 6.7: log Conductivity vs log System Size - Stationary GLE: The conductivities κ and κ° scale as N^{α}. The scaling coefficients α and α^{o} are reported in the legend for each temperature difference.


β^o vs T_R -T_L
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
β^o
-2
-1
0
1
2
3
4
5
6
Log(T_R -T_L)


β^o vs T_R -T_L
0.015
0.01
0.005
0
β^o
-2
-1
0
1
2
3
4
5
6
Log(T_R -T_L)

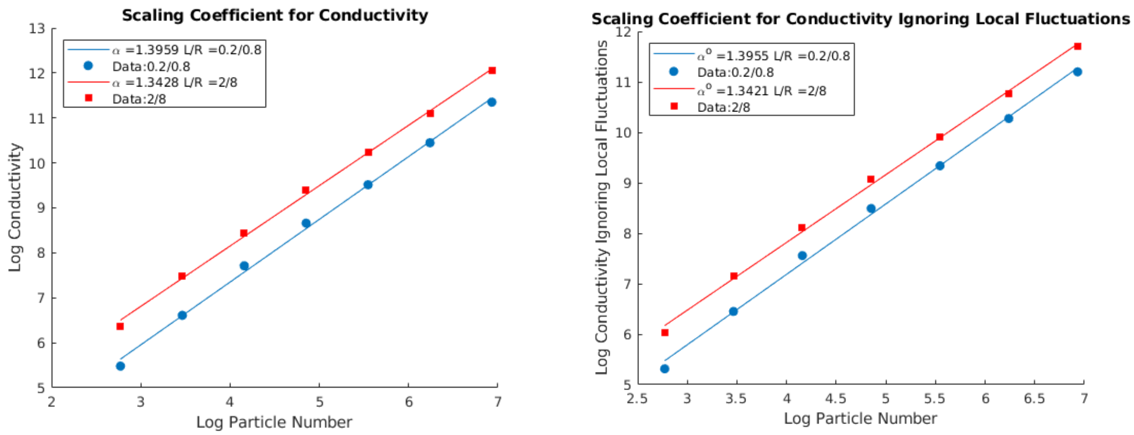


Figure 6.13: log Conductivity vs log System Size - Langevin Equation Free Boundary: The conductivities κ and κ° scale as N^α (resp. N^{α^o}) of the Langevin thermostat with free boundary condition. The scaling coefficient α is reported in the legend for each temperature difference.

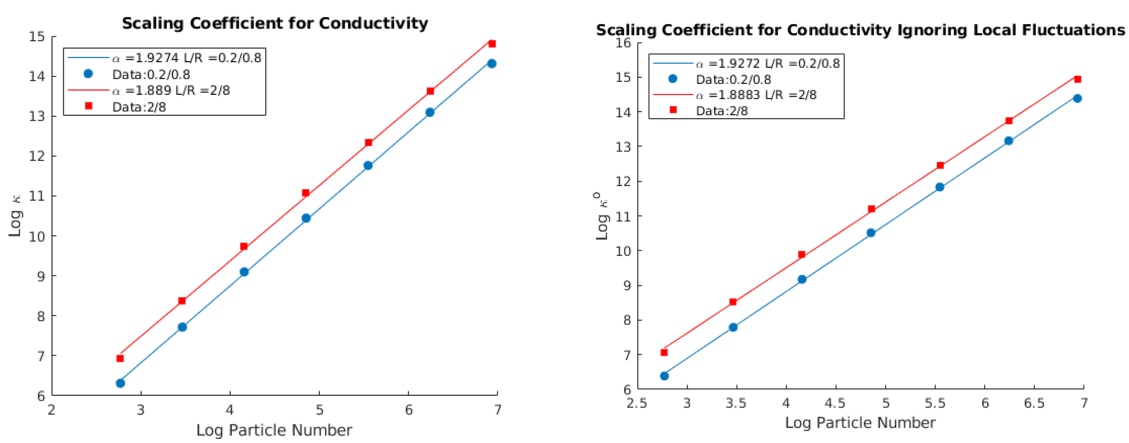


Figure 6.15: log Conductivity vs log System Size - Langevin equation Fixed Boundary: The conductivities κ and κ° scale as N^α (resp. N^{α^o}). The scaling coefficient α is reported in the legend for each temperature difference.

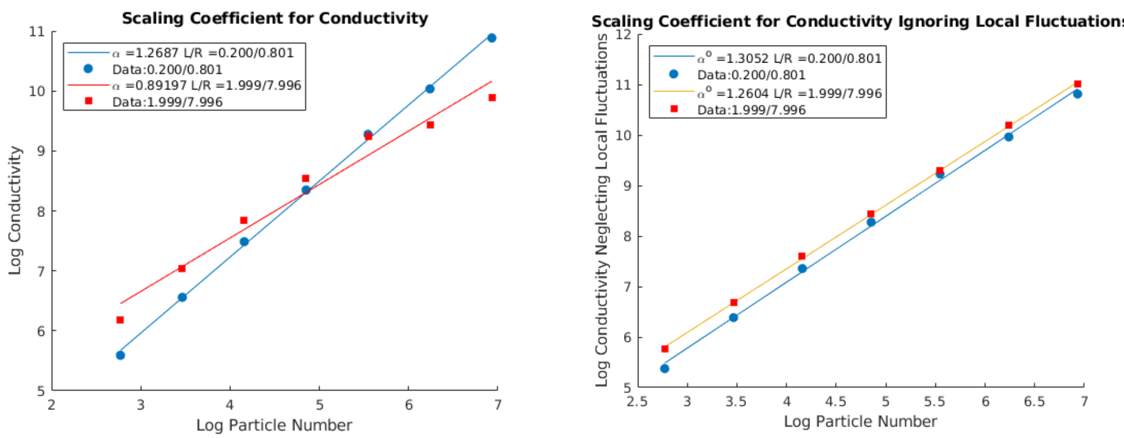
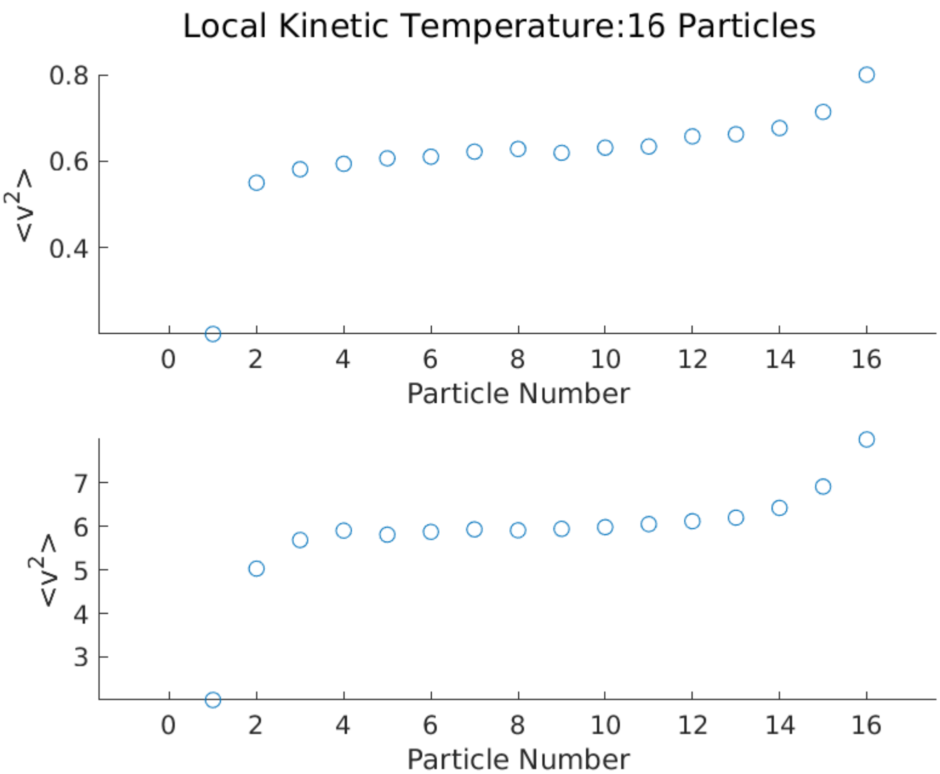
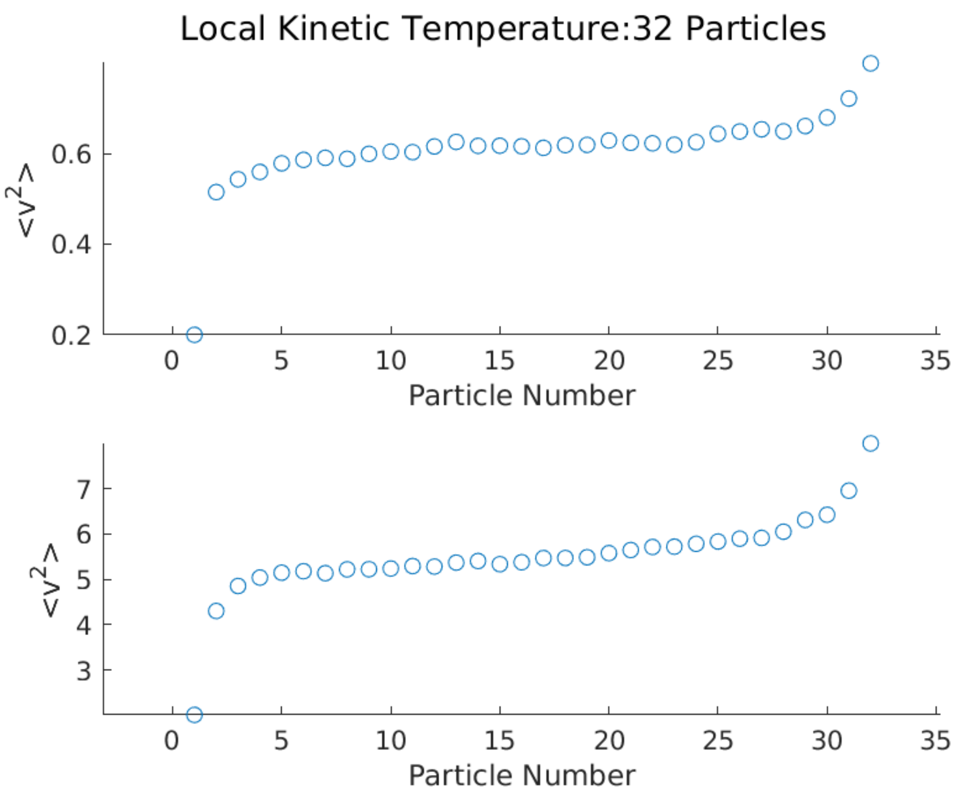


Figure 6.17: log Conductivity vs log System Size: The conductivities κ and κ° scale as N^α (resp. N^{α^o}). The scaling coefficient α is reported in the legend for each temperature difference.


Local Kinetic Temperature:16 Particles
<v^2>
0.8
0.6
0.4
0
2
4
6
8
10
12
14
16
Particle Number
<v^2>
7
6
5
4
3
0
2
4
6
8
10
12
14
16
Particle Number


Local Kinetic Temperature:32 Particles
<v^2>
0.6
0.4
0.2
0
5
10
15
20
25
30
35
Particle Number
<v^2>
7
6
5
4
3
0
5
10
15
20
25
30
35
Particle Number

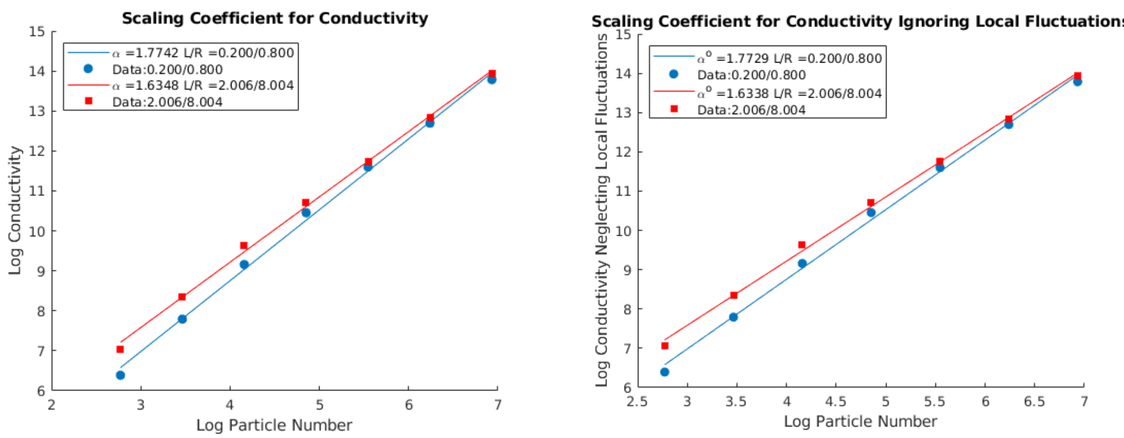


Figure 6.19: log Conductivity vs log System Size: The conductivities κ and κ° scale as N^{α} (resp. $N^{\alpha^{o}}$). The scaling coefficient α is reported in the legend for each temperature difference.

Chapter 7

Conclusion

By making the dimension reduction of the infinite determinstic bath thermostat rigorous through the use of Green's functions, it was discovered that the resulting noise term is non-stationary. To do this, we explicitly derived the covariance of semi-infinite deterministic equilibrium baths in theorem 2.10 on page 33. We showed that the statistics of the observables generated by position and momentum of the equilibrium measure remain invariant under time evolution of the equilibrium measure. In chapters 3 and 4 we solved for the Green's functions in Laplace space used them to prove the non-stationarity of the noise terms. This justifies the exact equivalence of the infinite deterministic system to the nonstationary GLE beginning at equation (6.15) on page 95. In chapter 5, we show that global in time solutions exist for equations similar to equation (6.15) on page 95, as well as Langevin type equations with a Lennard-Jones interaction potential. Finally in chapter 6, we investigate how to efficiently simulate GLE's. We approximate the memory kernel, as well as truncated versions of the memory kernel as a sum of exponentials. This allows for numerical integration of GLE's to be preformed much more efficiently. Different methods for computing the noise of the strong solution are investigated. Simulations of the stationary case, as well as other common thermostats is included.

The non-stationarity of the noise implied by Corollary 4.13 on page 75 provides both

T_L - T_R	Non-Stationary	Stationary	Langevin Free	Langevin Fixed	NH Free	NH Fixed
0.2 - 0.8	1.3579	1.3314	1.3955	1.9274	1.2687	1.7742
2 - 8	1.2055	1.1861	1.3431	1.889	1.3052	1.6348

Table 7.1: Conductivity Scaling: α for different thermostats and boundary conditions

theoretical and numerical challenges. If one could invert the difference calculated in Corollary 4.13, in principle one could have an analytic expression for the covariance of the noise in time domain. Analytic inversion of this term is challenging, and numerical inversion of the Laplace transform is an ill posed problem [10]. Another way to get such a value is to use the spectral representation of the noise to compute the covariance function directly. This way should allow for numerical computation, and possibly an analytic form, of the covariance function.

Table 7.1 lists the values of α for various thermostats at the warmer temperature configuration. From the table we see that assuming stationarity of the noise does affect the measured scaling coefficient α. Yet, the estimate provided by the weak approximation with stationary noise is much closer to the value computed with the non-stationary noise than the Nosé-Hoover or Langevin Thermostats with either fixed or free boundary conditions, which predict a faster rate of divergence for the conductivity.

The anomalous behavior of the temperature profile of the resolved system is strongly related to the chosen boundary conditions of the system. Fixed boundary conditions for the Langevin and Nosé-Hoover thermostats experience strong non-linear and discontinuous behavior even at high temperatures. Because the thermostats represented by the GLE's with non-stationary noise are the result of an exact dimension reduction technique, there is no need to specify additional boundary conditions. These systems only experience at most mild non-linear effects for most systems. When stationarity of the noise for the GLE is enforced, the non-linearity is enhanced for some systems, but again is damped for larger warmer systems. Free Langevin and Nosé-Hoover systems also experience only mild to no non-linear behavior for warmer larger systems, however the non-linearity present in these systems seems to have their own characteristic shape and these thermostats do not accurately predict the conductivity scaling coefficients α and α^o.

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